Supporting Information for

Ruthenium Olefin Metathesis Catalysts Bearing a *N*-fluorophenyl-*N*-mesityl-Substituted Unsymmetrical *N*-Heterocyclic Carbene

by

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Experimental Procedures

Materials and Methods:

All reactions involving metal complexes were conducted in oven-dried glassware under a nitrogen atmosphere with anhydrous solvents, using standard Schlenk and glovebox techniques. Anhydrous solvents were obtained via elution through a solvent column drying system.[1] Unless otherwise indicated, all compounds were purchased from Aldrich or Fisher. Catalyst **1** (Grubbs 1st generation) was obtained from Materia, Inc. Silica gel used for the purification of organometallic complexes was obtained from TSI Scientific, Cambridge, MA (60 Å, pH 6.5–7.0). NMR-Chemical shifts are reported in ppm downfield from Me_4Si, by using the residual solvent peak as internal standard for ^{1}H and ^{13}C, and H_3PO_4 (δ 0.0) for ^{31}P. Data for NMR spectra are reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz) and integration. Gas chromatography data was obtained using an Agilent 6850 FID gas chromatograph equipped with a DB-Wax Polyethylene Glycol capillary column (J&W Scientific). X-ray crystallographic structures were obtained by Mr. Larry M. Henling and Dr. Michael W. Day of the California Institute of Technology Beckman Institute X-ray Crystallography Laboratory. Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, U.K., and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition numbers 621770 (**5**) and 612854 (**6**). The screening of the catalysts, in ring-closing metathesis (RCM), cross metathesis (CM), and ring-opening metathesis polymerization reactions (ROMP), was conducted according to literature procedures.[2] The initiation kinetics studies were conducted according to literature procedures.[3]

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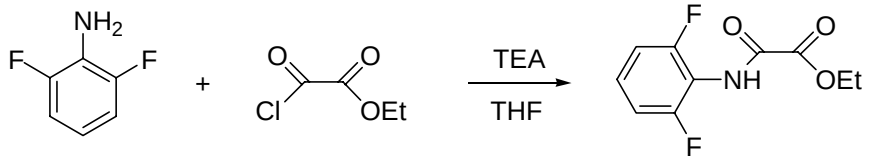
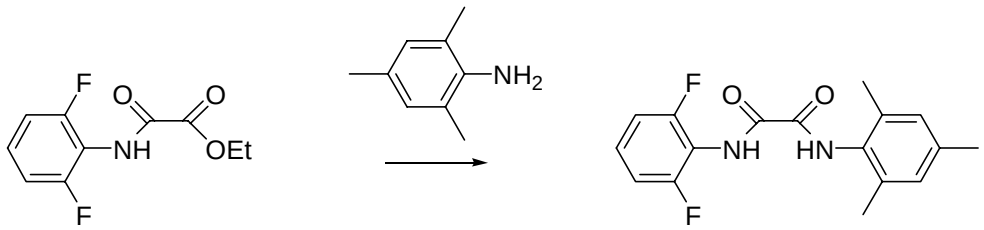
[1] Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518-1520.
[2] Ritter, T.; Hejl, A.; Wenzel, A. G.; Funk, T. W.; Grubbs, R. H. *Organometallics* **2006**, *25*, 5740-5745.
[3] Sanford, M. S.; Love, J. A.; Grubbs, R. H. *J. Am. Chem. Soc.* **2001**, *123*, 6543-6554.



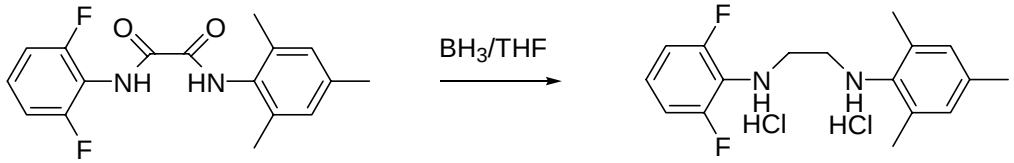
***N*-(2,6-difluorophenyl)-oxanilic acid ethyl ester (7).**

2,6-Difluoroaniline (10.11 mL, 100 mmol, 1.0 equiv.) and dry triethylamine (27.88 mL, 200 mmol, 2.0 equiv.) were dissolved in dry THF (200 mL) under nitrogen. This solution was cooled to 0 ^{o}C, and ethyl chlorooxoacetate (13.35 mL, 120 mmol, 1.2 equiv.) was added dropwise. Precipitation of a white solid (triethylamonium chloride) occurred immediately upon addition. The suspension was allowed to stir for 16 h, warming to room temperature. The solid was filtered off and washed with diethyl ether (200 mL), and the combined organic layer was washed with an aqueous saturated NH_4Cl solution until pH 6. This organic layer was then washed with brine (150 mL) and dried over $MgSO_4$. The solvent was removed under reduced pressure leaving a yellow solid that was washed with hexanes (3 × 6 mL) to afford a yellowish crystalline solid (19.94 g, 87 mmol, 87% yield). ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 8.46 (broad s, 1H), 7.30–7.26 (m, 1H), 7.03–6.99 (m, 2H), 4.45 (q, J = 7 Hz, 2H), 1.45 (t, J = 7 Hz, 3H); ^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz): δ = 159.76 (s), 157.42 (dd, $^{1}J_{CF}$ = 253 Hz, $^{3}J_{CF}$ = 5 Hz), 154.44 (s), 128.44 (t, $^{3}J_{CF}$ = 10 Hz), 112.21 (t, $^{2}J_{CF}$ = 17 Hz), 111.73 (dd, $^{2}J_{CF}$ = 19 Hz, $^{4}J_{CF}$ = 4 Hz), 63.57 (s), 13.72 (s); ^{19}F{^{1}H} NMR ($CDCl_3$, 169 MHz): δ = -117.22 (s); HRMS (FAB^{+}) calculated for $C_{10}H_{10}NO_3F_2$ $[M]^{+}$ 230.0629, observed 230.0621.



***N*-(2,6-difluorophenyl)-*N'*-(mesityl)-oxalamide (8).**

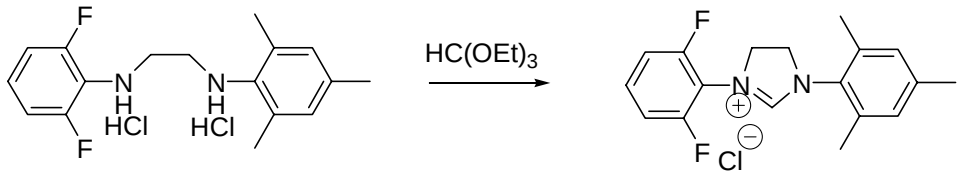
N-(2,6-difluoro)-oxanilic acid ethyl ester (**7**) (8.887 g, 40 mmol, 1.0 equiv.) was dissolved in 2,4,6-trimethylaniline (10.1 mL, 72 mmol, 1.8 equiv.) in a dry Schlenk tube under nitrogen. The tube was sealed and the suspension was stirred at 180 ^{o}C for 16 h. Upon being cooled to room temperature, the reaction mixture solidified. The brownish solid was washed with hexanes (3 × 20 mL) and diethyl ether (3 × 5 mL), leaving an off-white solid (6.621 g, 21 mmol, 52% yield). ^{1}H NMR ($CDCl_3$, 300 MHz): δ = 8.91 (broad s, 1H), 8.70 (broad s, 1H), 7.32–7.28 (m, 1H), 7.05–7.01 (m, 2H), 6.94 (s, 2H), 2.30 (s, 3H), 2.24 (s, 6H); ^{13}C{^{1}H} NMR ($CDCl_3$, 125 MHz): δ = 165.42 (s), 159.86 (s), 157.72 (dd, $^{1}J_{CF}$ = 253 Hz, $^{3}J_{CF}$ = 5 Hz), 157.52 (s), 137.95 (s), 134.95 (s), 129.31 (s), 128.66 (t, $^{3}J_{CF}$ = 10 Hz), 112.74 (t, $^{2}J_{CF}$ = 17 Hz), 112.19 (dd, $^{2}J_{CF}$ = 19 Hz, $^{4}J_{CF}$ = 4 Hz), 21.19 (s), 18.59 (s); ^{19}F{^{1}H} NMR ($CDCl_3$, 169 MHz): δ = -117.07 (s); HRMS (FAB^{+}) calculated for $C_{17}H_{17}N_2O_2F_2$ $[M]^{+}$ 319.1258, observed 319.1269.



***N*-(2,6-difluorophenyl)-*N'*-(mesityl)-1,2-ethanediamine dihydrochloride (9).**

In a dry, high pressure tube containing *N*-(2,6-difluoro)-*N'*-(mesityl)-oxalamide (**8**) (6.366 g, 20 mmol, 1.0 equiv.) was added BH_3•THF (1 M in THF) (100 mL, 100 mmol, 5 equiv.) under

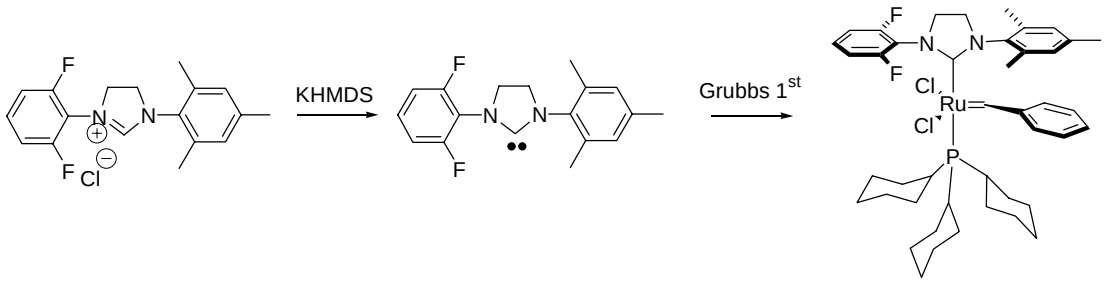
nitrogen. The tube was sealed and the solution was stirred at 75 °C for 16 h. Upon being cooled to room temperature, the clear yellowish solution was slowly added to methanol (200 mL) at 0 °C. Concentrated HCl solution (4.92 mL) was also slowly added at 0 °C. When all bubbling ceased, the solvent was removed under reduced pressure. The resulting solid was dissolved in methanol and the solvent was again removed under reduced pressure. This was repeated twice more to remove the remaining boron as $B(OMe)_3$. The remaining white solid was finally washed with diethyl ether (2 × 10 mL) to provide the desired product as a white solid (4.181 g , 14.4 mmol, 72% yield). ^{1}H NMR (DMSO-d_6, 300 MHz): δ = 7.00–6.90 (m, 4H), 6.74–6.64 (m, 1H), 3.73–3.68 (m, 2H), 3.41–3.37 (m, 2H), 2.43 (s, 6H), 2.22 (s, 3H); ^{13}C{^{1}H} NMR (DMSO-d_6, 125 MHz): δ = 152.26 (dd, $^1J_{CF}$ = 240 Hz, $^3J_{CF}$ = 8 Hz), 138.26 (s), 131.82 (s), 130.31 (s), 124.80 (t, $^3J_{CF}$ = 13 Hz), 116.97 (t, $^2J_{CF}$ = 10 Hz), 111.77 (dd, $^2J_{CF}$ = 17 Hz, $^4J_{CF}$ = 6 Hz), 50.51 (s), 41.35 (s), 20.14 (s), 17.63 (s); ^{19}F{^{1}H} NMR ($CDCl_3$, 169 MHz): δ = -128.72 (s); HRMS (FAB$^+$) calculated for $C_{17}H_{21}N_2F_2$ $[M]^+$ 291.1673, observed 291.1672.



1-(2,6-difluorophenyl)-3-(mesityl)-4,5-dihydro-imidazolium chloride (10).

A suspension of *N*-(2,6-difluorophenyl)-*N'*-(mesityl)-1,2-ethanediamine dihydrochloride (**9**) (2.180 g, 6 mmol, 1.0 equiv.) in triethylorthoformate (19.95 mL, 120 mmol, 20 equiv.) was heated at 135 °C for 30 min under nitrogen. After cooling to room temperature, the solids were filtered of and washed with diethyl ether (3 × 15 mL) to provide the desired product as a white solid (1.878 g , 5.6 mmol, 93% yield). ^{1}H NMR (DMSO-d_6, 300 MHz): δ = 9.42 (s, 1H), 7.67–

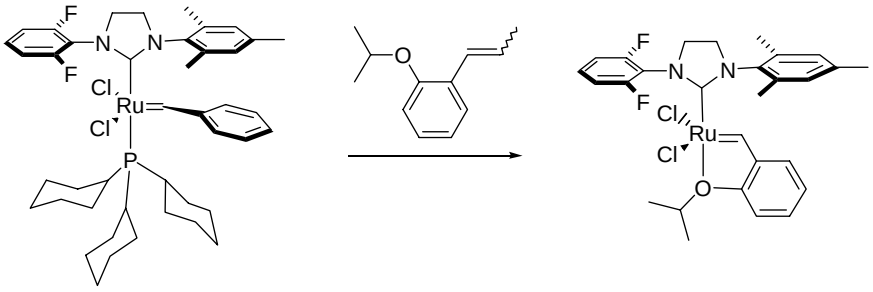
7.57 (m, 1H), 7.47–7.41 (m, 2H), 7.10 (s, 2H), 4.67–4.60 (m, 2H), 4.49–4.42 (m, 2H), 2.33 (s, 6H), 2.29 (s, 3H); $^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 125 MHz): δ = 160.89 (s), 156.48 (dd, $^{1}J_{CF}$ = 252 Hz, $^{3}J_{CF}$ = 3 Hz), 139.73 (s), 134.99 (s), 130.96 (t, $^{3}J_{CF}$ = 10 Hz), 130.54 (s), 129.37 (s), 113.53 (t, $^{2}J_{CF}$ = 15 Hz), 112.88 (dd, $^{2}J_{CF}$ = 19 Hz, $^{4}J_{CF}$ = 4 Hz), 51.40 (s), 51.31 (s), 20.45 (s), 17.01 (s); $^{19}F\{^{1}H\}$ NMR ($CDCl_3$, 169 MHz): δ = -119.84 (s); HRMS (FAB^+) calculated for $C_{21}H_{25}F_2N_2$ $[M]^+$ 343.1986, observed 343.1987.



[$RuCl_2$ (1-(2,6-difluorophenyl)-3-mesityl-dihydroimidazol-ylidene) (=CH-Ph) (PCy_3)] (5).

1-(2,6-difluorophenyl)-3-(mesityl)-4,5-dihydro-imidazolium chloride (**10**) (337 mg, 1 mmol, 2.0 equiv.) was stirred with an equimolar quantity of KHMDS in benzene (10 mL, 0.1 M) in a glove box at room temperature for 45 min. Catalyst **1** (411 mg, 0.5 mmol, 1.0 equiv.) was added as a solid in one portion, the reaction flask was taken out of the glove box and heated under a nitrogen atmosphere at 80 ^{o}C for 30 min. The solution was concentrated to 2 mL in vacuo and poured onto a column packed with TSI Scientific silica gel. The complex was eluted with hexanes/diethyl ether (2/1) as a red band. This was concentrated in vacuo, transferred in a glove box, dissolved in the minimum amount of benzene and lyophilized to afford the desired complex as a violet-dark red solid (350 mg, 0.41 mmol, 83% yield). The solid is stable in air in the solid state and soluble in CH_2Cl_2, $CHCl_3$, benzene, toluene and THF. Crystals suitable for X-ray

crystallography were grown at room temperature by slow diffusion of hexanes into a solution of **5** in benzene. ^{1}H NMR (CD_2Cl_2, 500 MHz): δ = 19.42 (s, 1H–minor), 19.14 (s, 1H–major), 7.47–7.37 (m, 2H–major, 2H–minor), 7.14–7.09 (m, 4H–major), 7.01 (s, 2H–minor), 6.75–6.72 (m, 1H–minor), 4.12–3.89 (m, 4H–major, 4H–minor), 2.63–0.90 (m, 42H–major, 42H–minor); $^{13}C\{^{1}H\}$ NMR (CD_2Cl_2, 125 MHz, due to extensive fluorine coupling and the existence of two rotational isomers, some coupling constants are not given): δ = 297.52–297.32 (m, major), 294.67–294.47 (m, minor), 223.88 (s), 223.40 (s), 223.27 (s), 222.77 (s), 161.36 (dd, $^{1}J_{CF}$ = 256 Hz, $^{3}J_{CF}$ = 4 Hz, major), 159.84 (dd, $^{1}J_{CF}$ = 252 Hz, $^{3}J_{CF}$ = 3 Hz, minor), 152.06 (s), 151.25 (s), 138.77 (s), 138.14 (s), 136.89 (s), 136.72 (s), 135.24 (s), 131.28 (t, $^{3}J_{CF}$ = 10 Hz, major), 130.20 (s), 129.98 (s), 129.68 (t, $^{3}J_{CF}$ = 10 Hz, minor), 129.16 (s), 128.67 (s), 128.42 (s), 127.93 (s), 112.69 (dd, $^{2}J_{CF}$ = 20 Hz, $^{4}J_{CF}$ = 3 Hz, major), 111.82 (dd, minor), 53.17 (s), 53.14 (s), 53.03 (s), 53.00 (s), 52.15 (s), 52.13 (s), 35.71 (s), 35.23 (s), 32.02 (s), 31.90 (s), 31.76 (s), 28.01 (s), 27.96 (s), 27.93 (s), 27.88 (s), 27.21 (s), 27.11 (s), 26.57 (s), 26.55 (s), 26.45 (s), 26.44 (s), 26.41 (s), 26.36 (s), 21.07 (s), 20.87 (s), 19.71 (s), 18.33 (s); $^{31}P\{^{1}H\}$ NMR (CD_2Cl_2, 202 MHz) δ = 31.54 (s, minor), 27.54 (s, major); $^{19}F\{^{1}H\}$ NMR (CD_2Cl_2, 282 MHz): δ = -103.20 (s, major), -125.15 (s, minor); HRMS (FAB^{+}) calculated for $C_{43}H_{57}N_2F_2Cl_2PRu$ $[M]^{+}$ 842.2649, observed 842.2681; Anal. calculated for $C_{43}H_{57}N_2F_2Cl_2PRu$: 61.27 C, 6.82 H, 3.32 N. Found: 61.51 C, 7.08 H, 3.31 N.



[$RuCl_2$ (1-(2,6-difluorophenyl)-3-mesityl-dihydroimidazol-ylidene) (=CH-*o*-*i*PrO-Ph)] (6).

In a glovebox, a vial was charged with complex **5** (169 mg, 0.2 mmol, 1.0 equiv.), toluene (8 mL, 0.025 M) and *o*-isopropoxy-*β*-methylstyrene (175 mg, 4 mmol, 20.0 equiv.). The dark red solution was stirred for 10 min and then left inside the capped vial without stirring. After 40 h at room temperature, the desired complex had precipitated as dark green crystals. The supernatant brown liquid was decanted off; the crystals were washed with hexanes (2 × 10 mL) and dried in vacuo to afford (92 mg, 0.15 mmol, 74% yield). The solid is stable in air in the solid state and soluble in CH_2Cl_2, $CHCl_3$ and benzene. The crystals obtained from the above procedure (preparation of the complex) were suitable for X-ray crystallography. ^{1}H NMR (CD_2Cl_2, 500 MHz): δ = 16.14 (s, 1H), 7.57–7.45 (m, 2H), 7.15–7.09 (m, 4H), 6.95–6.86 (m, 3H), 4.96 (septet, 1H, J_{HH} = 6 Hz), 4.30–4.15 (m, 4H), 2.46 (s, 3H), 2.31 (s, 6H), 1.30 (d, J_{HH} = 6 Hz, 6H); ^{13}C{^{1}H} NMR (CD_2Cl_2, 125 MHz): δ = 292.59 (d, J = 29 Hz), 215.29 (s), 162.02 (dd, $^1J_{CF}$ = 255 Hz, $^3J_{CF}$ = 4 Hz), 152.73 (s), 144.94 (s), 139.69 (s), 138.33 (s), 137.94 (s), 131.51 (t, $^3J_{CF}$ = 10 Hz), 130.14 (s), 130.12 (s), 129.49 (s), 128.68 (s), 122.90 (s), 122.79 (s), 118.11 (t, $^1J_{CF}$ = 15 Hz) 113.41 (s), 112.79 (dd, $^2J_{CF}$ = 20 Hz, $^4J_{CF}$ = 5 Hz), 75.77 (s), 53.42 (s), 52.23 (s), 21.60 (s), 21.48 (s), 18.33 (s); ^{19}F{^{1}H} NMR (CD_2Cl_2, 282 MHz): δ = -108.28 (s); HRMS (FAB$^+$) calculated for $C_{28}H_{30}N_2OF_2Cl_2Ru$ $[M]^+$ 620.0747, observed 620.0767; Anal. calculated for $C_{28}H_{30}N_2OF_2Cl_2Ru$: 54.20 C, 4.87 H, 4.51 N. Found: 54.13 C, 4.71 H, 3.92 N.

Line Shape and Eyring Analysis

For the variable-temperature NMR experiments the probe was calibrated at each temperature with a glycol standard for each measurement. NMR spectral simulations were performed using gNMR version 3.6. The chemical shifts observed in the slow limit exchange (298 K) were used to set up the spin systems. Lorentzian lineshapes with linewidths of 2 Hz were utilized. Small changes to the linewidth did not affect the activation parameters of the exchange process. As the chemical shifts of the different hydrogens vary slightly with temperature, the difference in the chemical shifts was used to compare simulated with experimental spectra. For different temperatures, the exchange rate was varied to get the best fit between the simulated and the experimental spectra. An Eyring plot for data collected over the range 323–378 K was used to extract the entropy and enthalpy of activation from the temperature dependence of the rate constant (Figure S1).The experimental as well as the simulated NMR spectra are presented in Figure S2.

$\Delta H^{\ddagger}$ (kcal/mol)	$\Delta S^{\ddagger}$ (cal/(mol•K))	$\Delta G^{\ddagger}$ (298K) (kcal/mol)
19.6±0.7	**6±2**	**17.9±0.1**

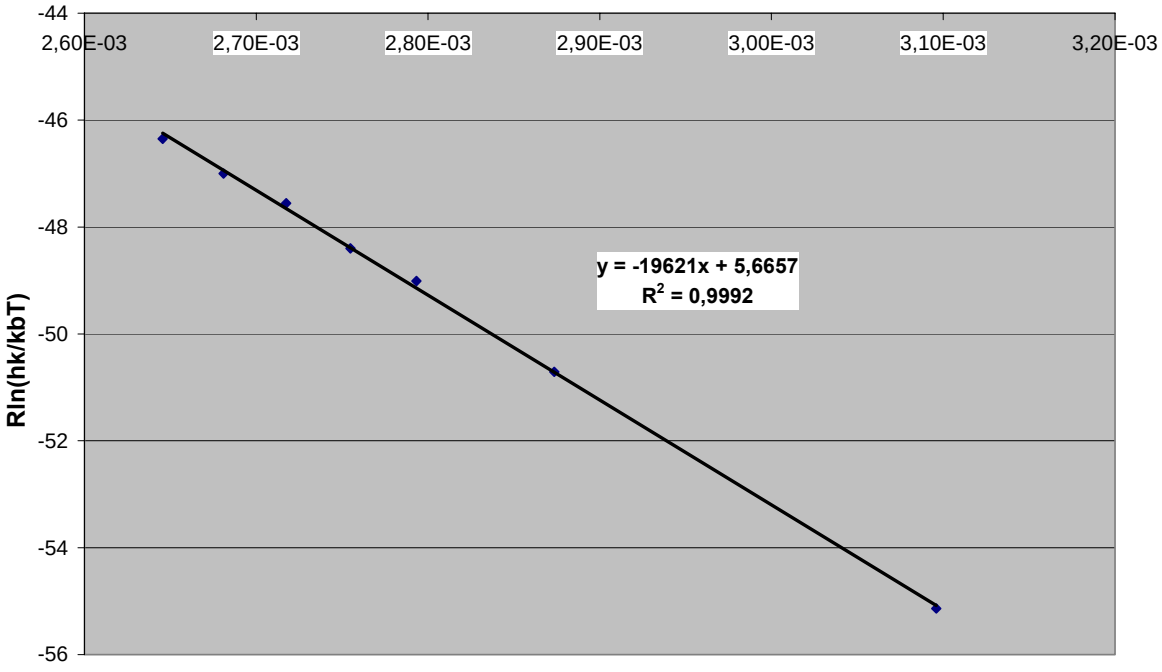


Figure S1.

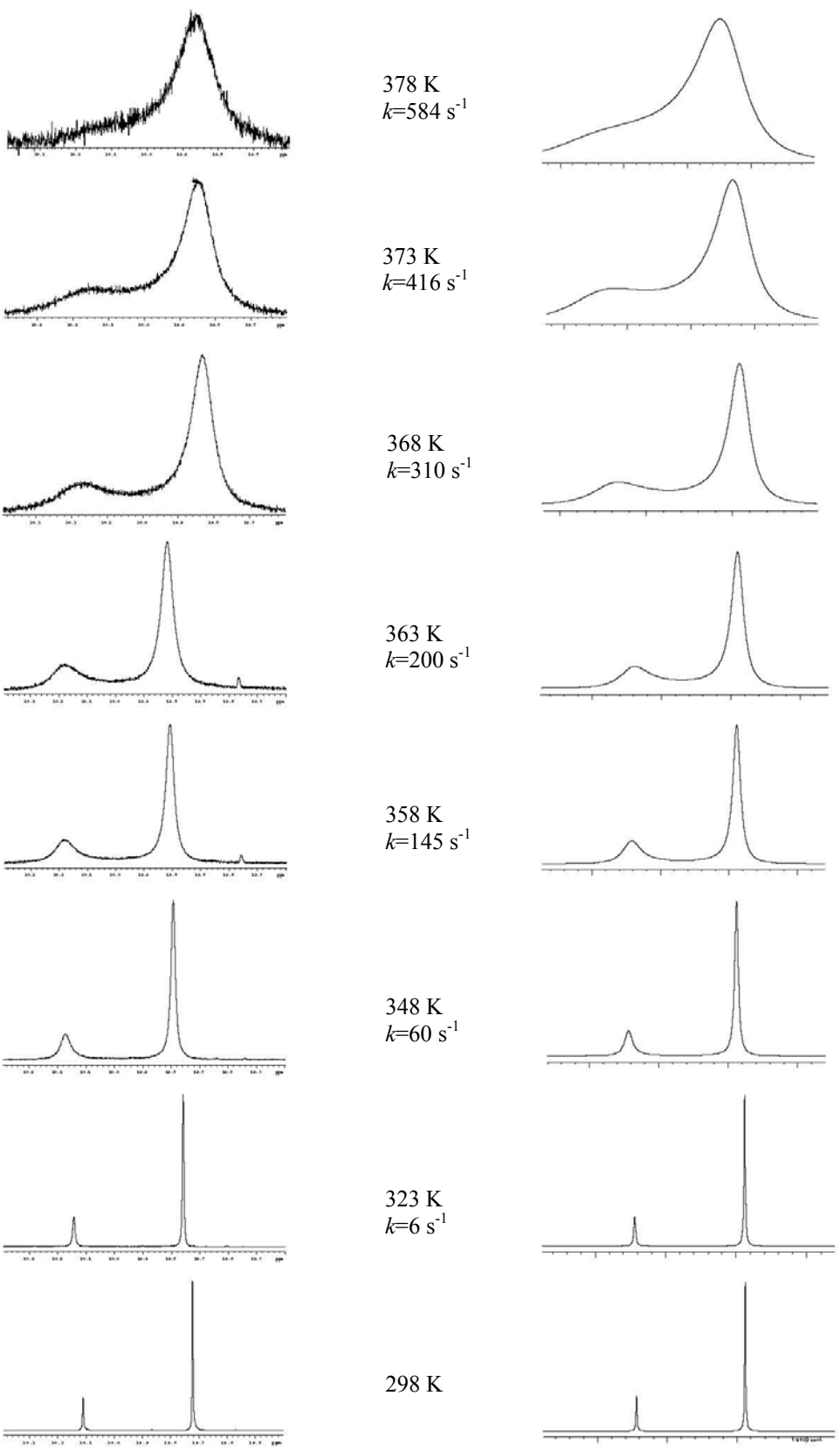
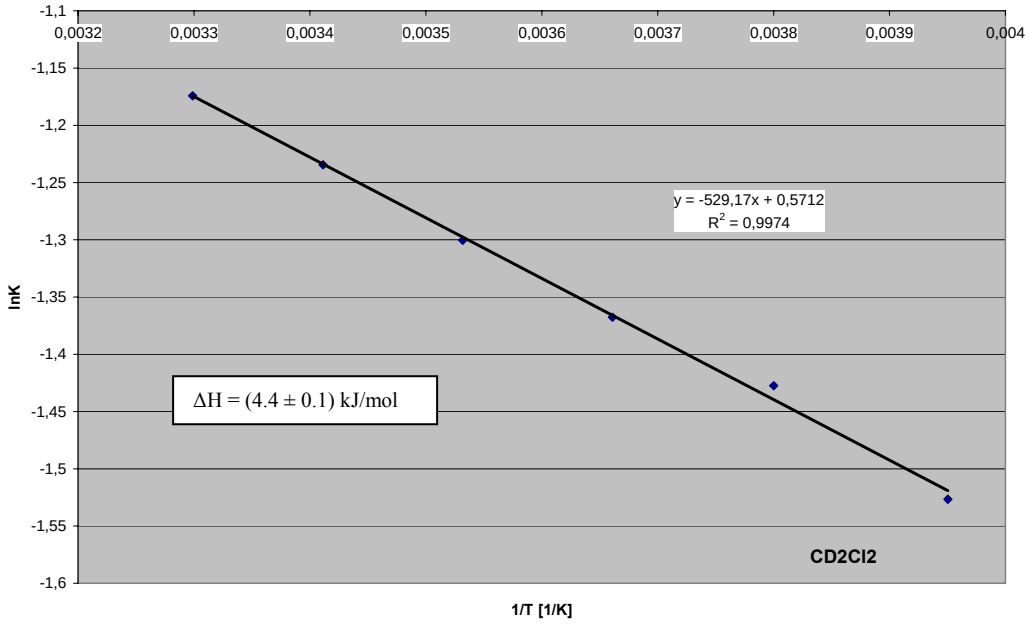
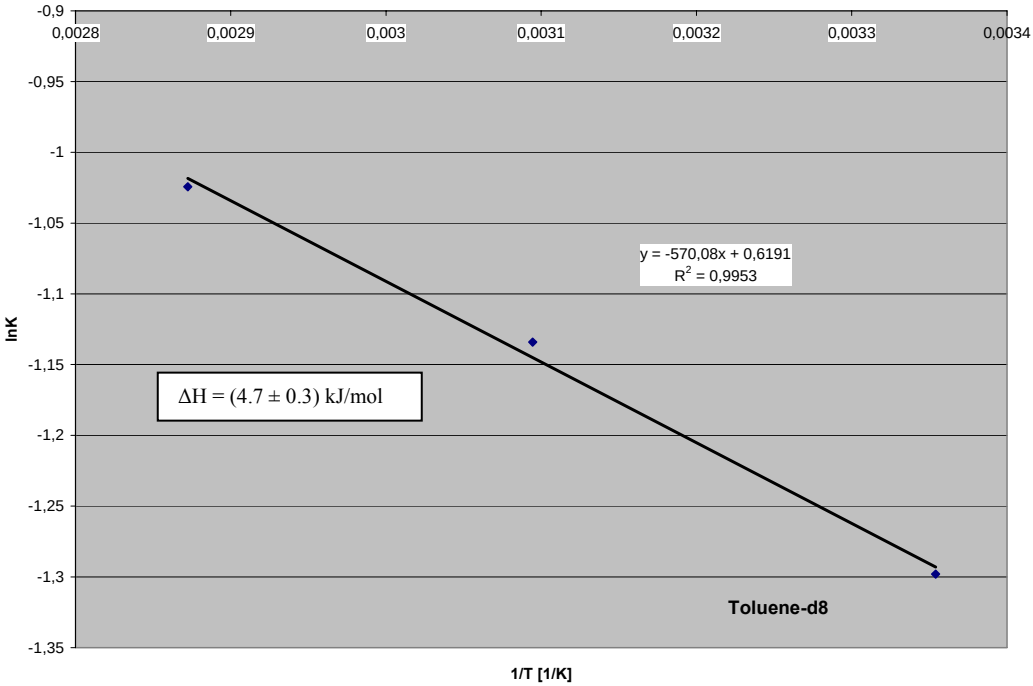

Experimental Spectra
Simulated Spectra
378 K
k=584 s-1
373 K
k=416 s-1
368 K
k=310 s-1
363 K
k=200 s-1
358 K
k=145 s-1
348 K
k=60 s-1
323 K
k=6 s-1
298 K

Figure S2.

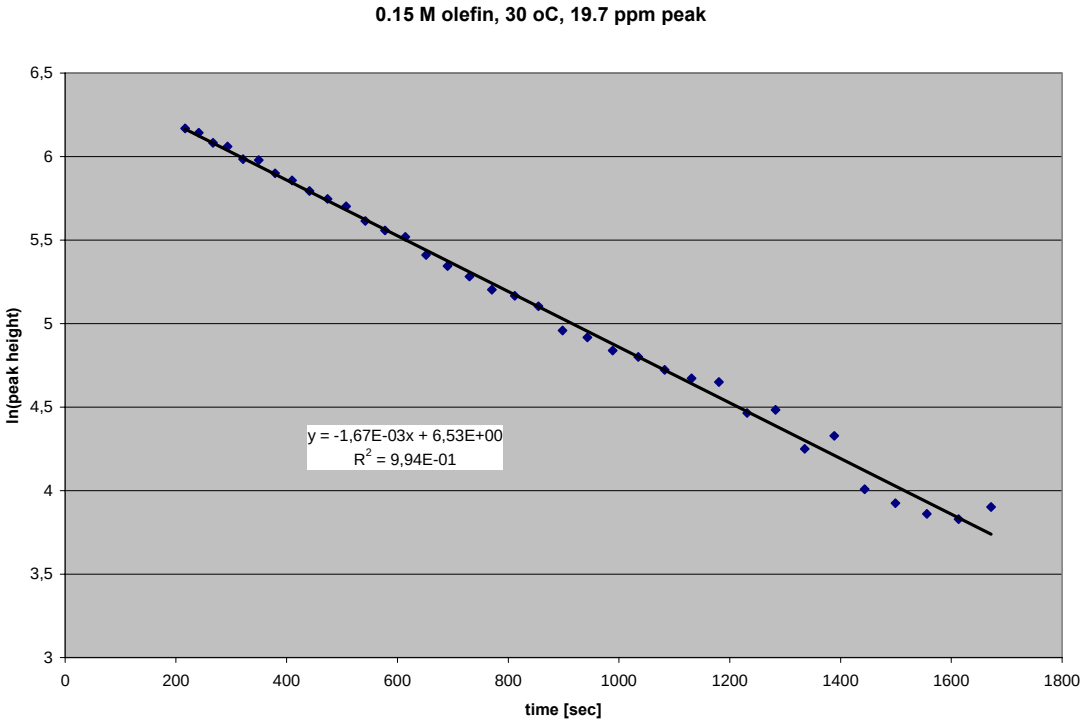
Temperature Dependence of the Equilibrium Constant for the two Rotamers of Catalyst 5.

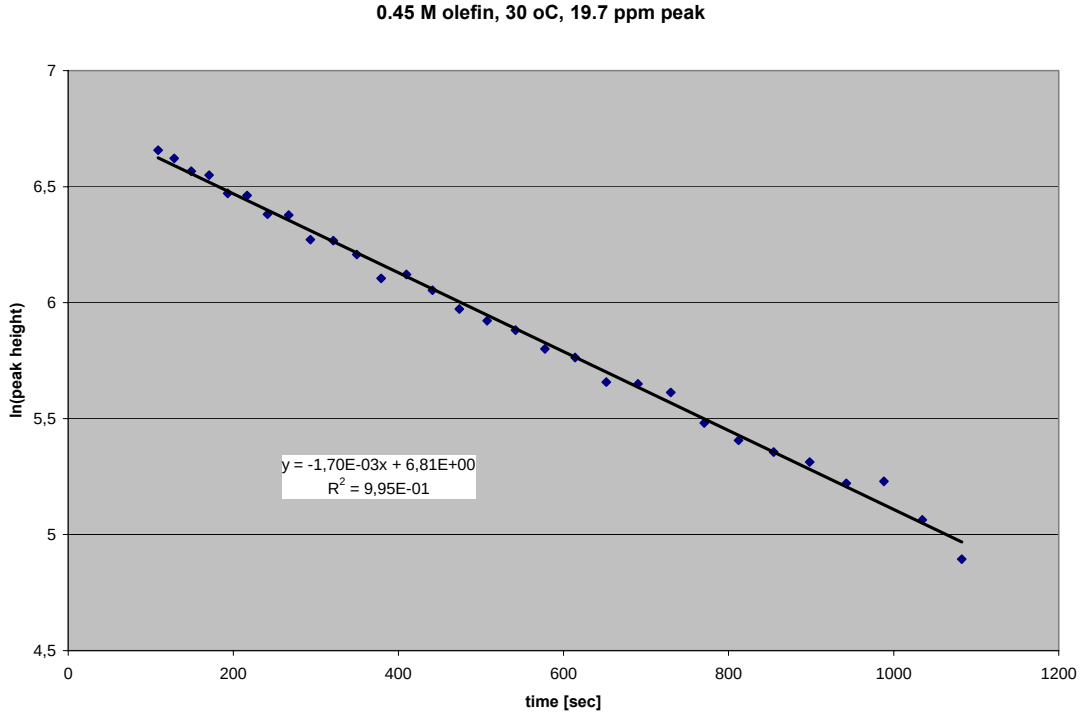


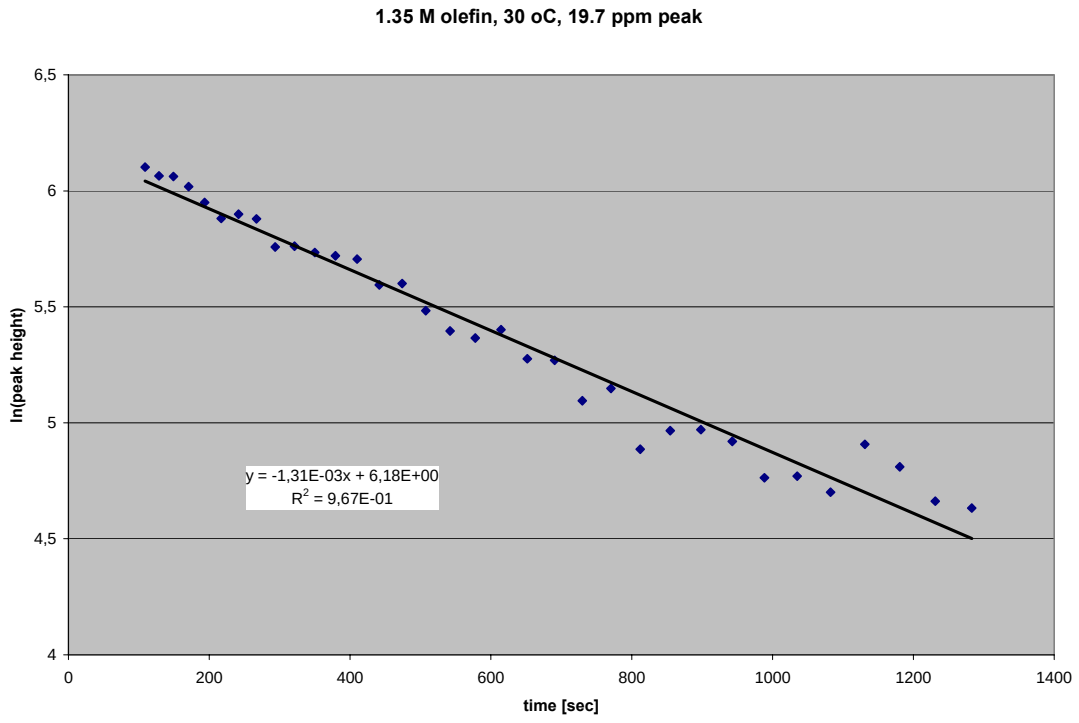


Initiation Kinetics Experiments

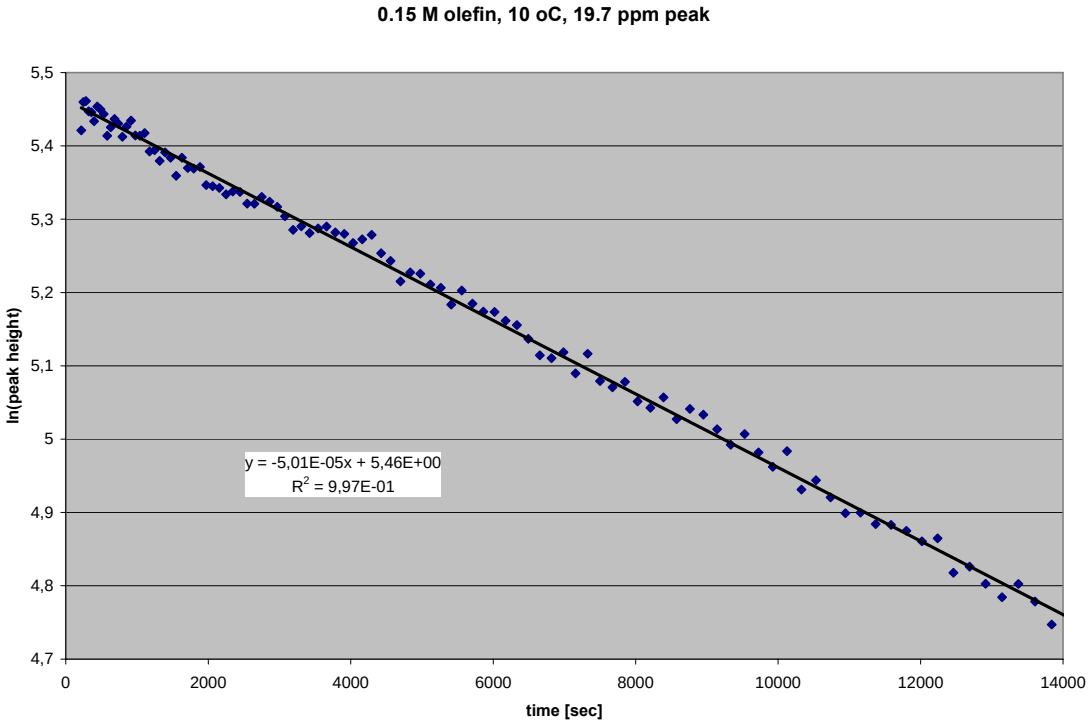
a) Initiation rate constant dependence on olefin concentration



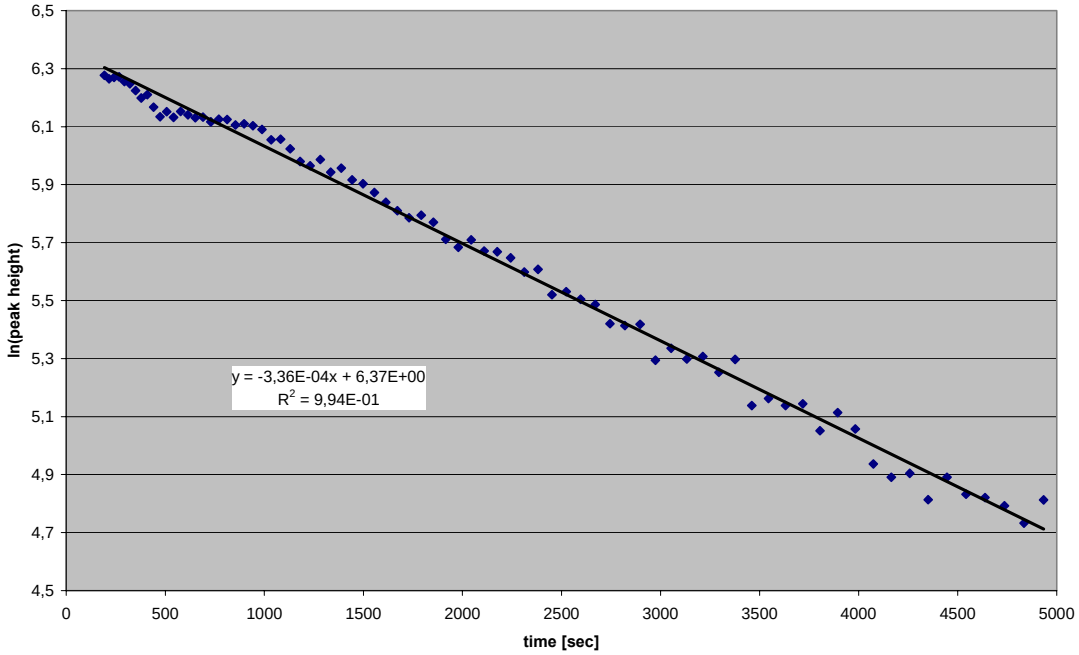




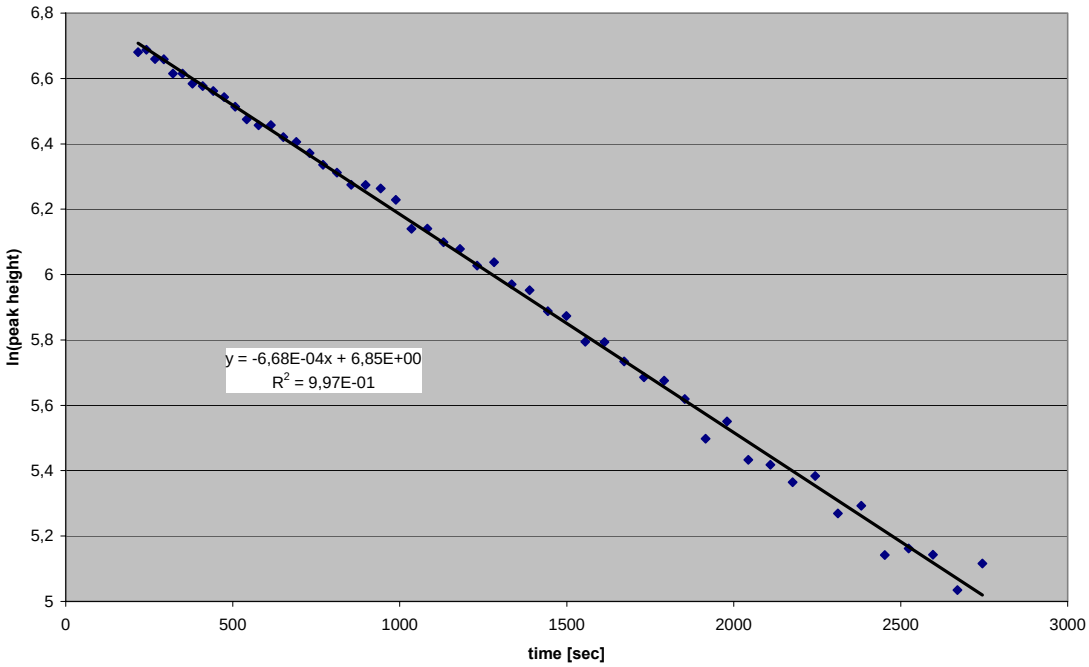
b) Initiation rate constant dependence on temperature



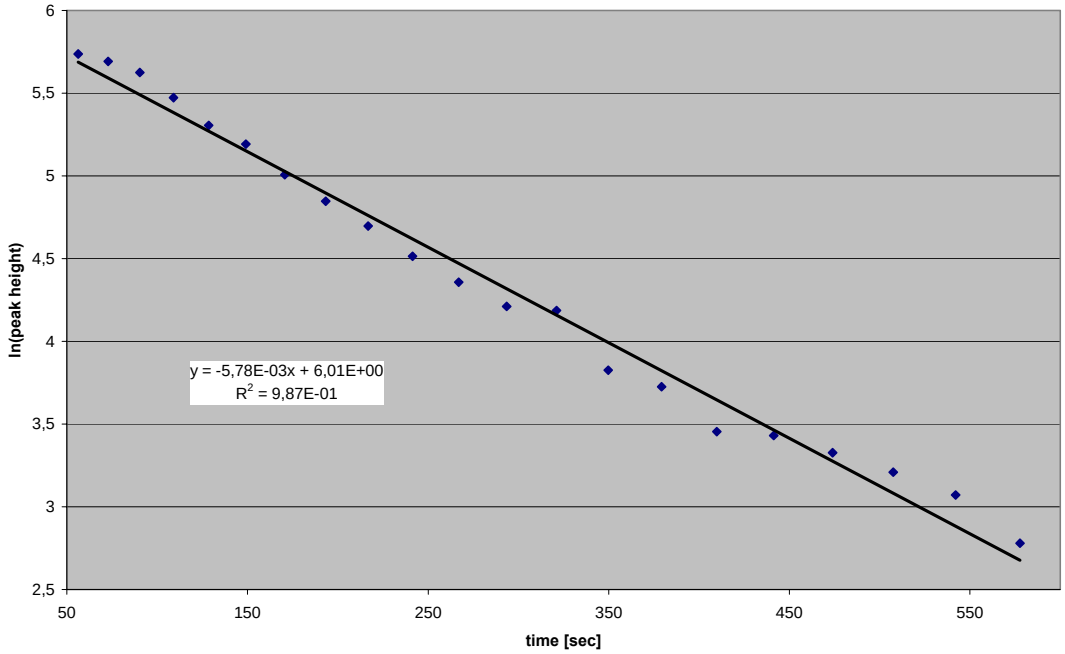
0.15 M olefin, 20 oC, 19.7 ppm peak



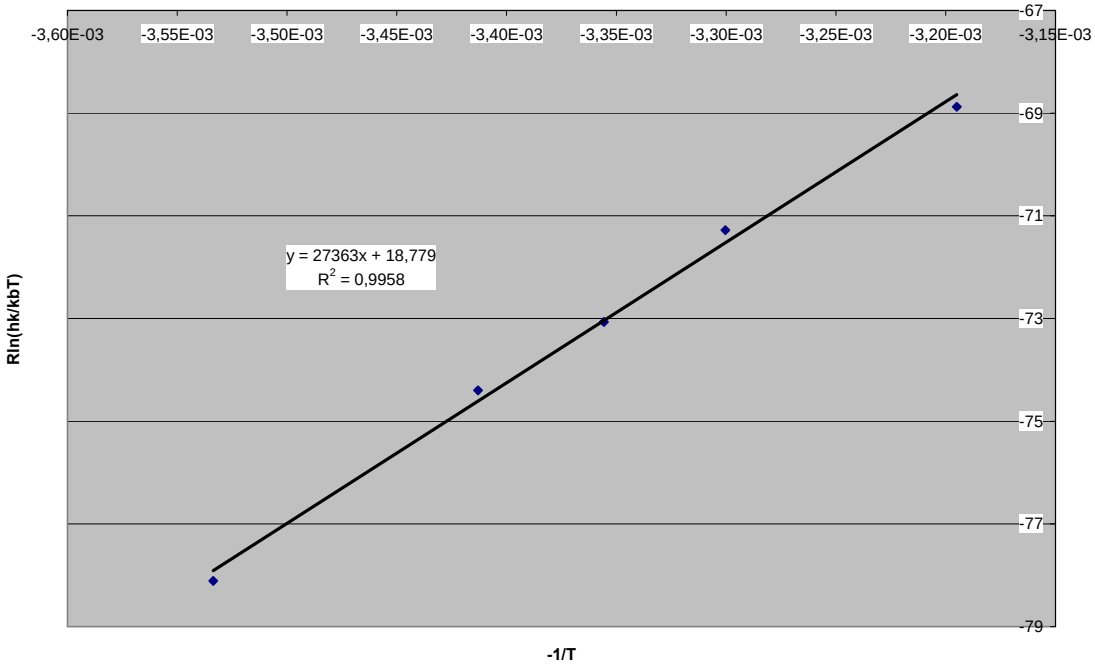
0.15 M olefin, 25 oC, 19.7 ppm peak



0.15 M olefin, 40 oC, 19.7 ppm peak



Eyring Plot (Temp. Dep. of kobs)



Crystallographic Analysis

[$RuCl_2$ (1-(2,6-difluorophenyl)-3-mesityl-dihydroimidazol-ylidene) (=CH-Ph) (PCy_3)] (5)

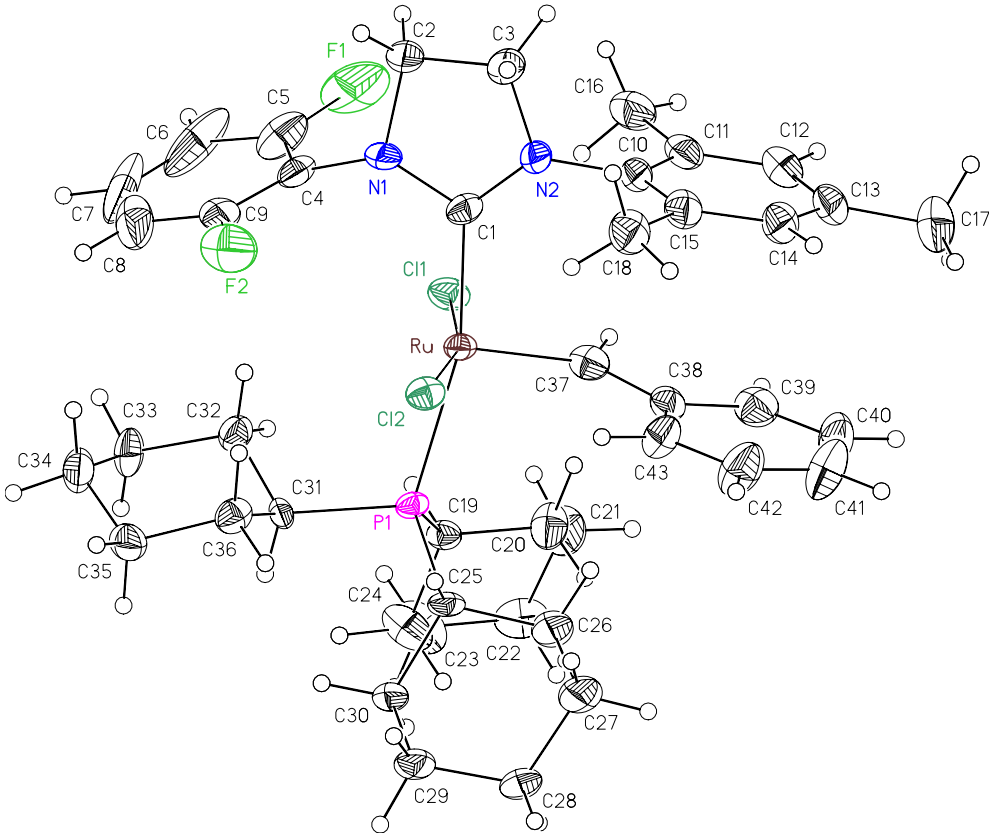


Table 1. Crystal data and structure refinement for CCDC 621770.

Empirical formula	$C_{43}H_{57}F_2N_2PCl_2Ru$
Formula weight	842.85
Crystallization Solvent	Toluene
Crystal Habit	Fragment
Crystal size	0.37 x 0.36 x 0.23 mm^3
Crystal color	Dark purple

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 26002 reflections used in lattice determination	2.42 to 33.23°
Unit cell dimensions	a = 25.2082(12) Å b = 9.8032(5) Å c = 16.0304(8) Å
Volume	3961.4(3) $Å^3$
Z	4
Crystal system	Orthorhombic
Space group	$Pna2_1$
Density (calculated)	1.413 Mg/m^3
F(000)	1760
Data collection program	Bruker SMART v5.630
θ range for data collection	1.62 to 33.90°
Completeness to θ = 33.90°	92.8 %
Index ranges	$-38 \le h \le 38$, $-14 \le k \le 14$, $-24 \le l \le 24$
Data collection scan type	ω scans at 5 ϕ settings
Data reduction program	Bruker SAINT v6.45A
Reflections collected	65856
Independent reflections	14331 [R_{int}= 0.0892]
Absorption coefficient	0.614 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.8717 and 0.8048

Table 1 (cont.)

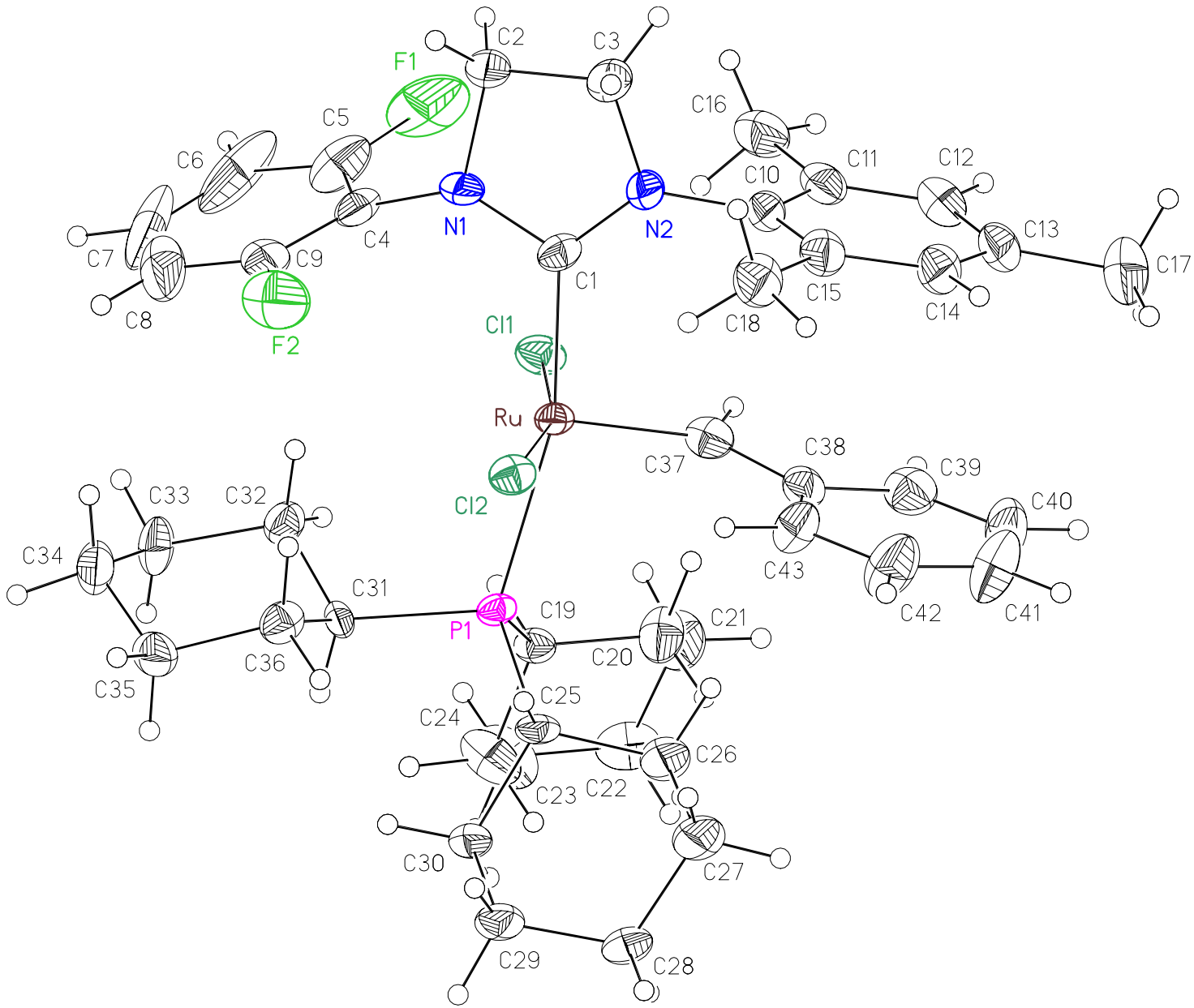
Structure solution and Refinement

Structure solution program	Bruker XS v6.12
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	14331 / 1 / 463
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.823
Final R indices [$I>2\sigma(I)$, 10845 reflections]	R1 = 0.0607, *w*R2 = 0.0978
R indices (all data)	R1 = 0.0864, *w*R2 = 0.1016
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Absolute structure determination	Anomalous dispersion
Absolute structure parameter	-0.02(3)
Largest diff. peak and hole	4.072 and -1.723 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C2
C3
F1
C5
C16
C6
C10
C11
C12
C4
N1
N2
C13
C7
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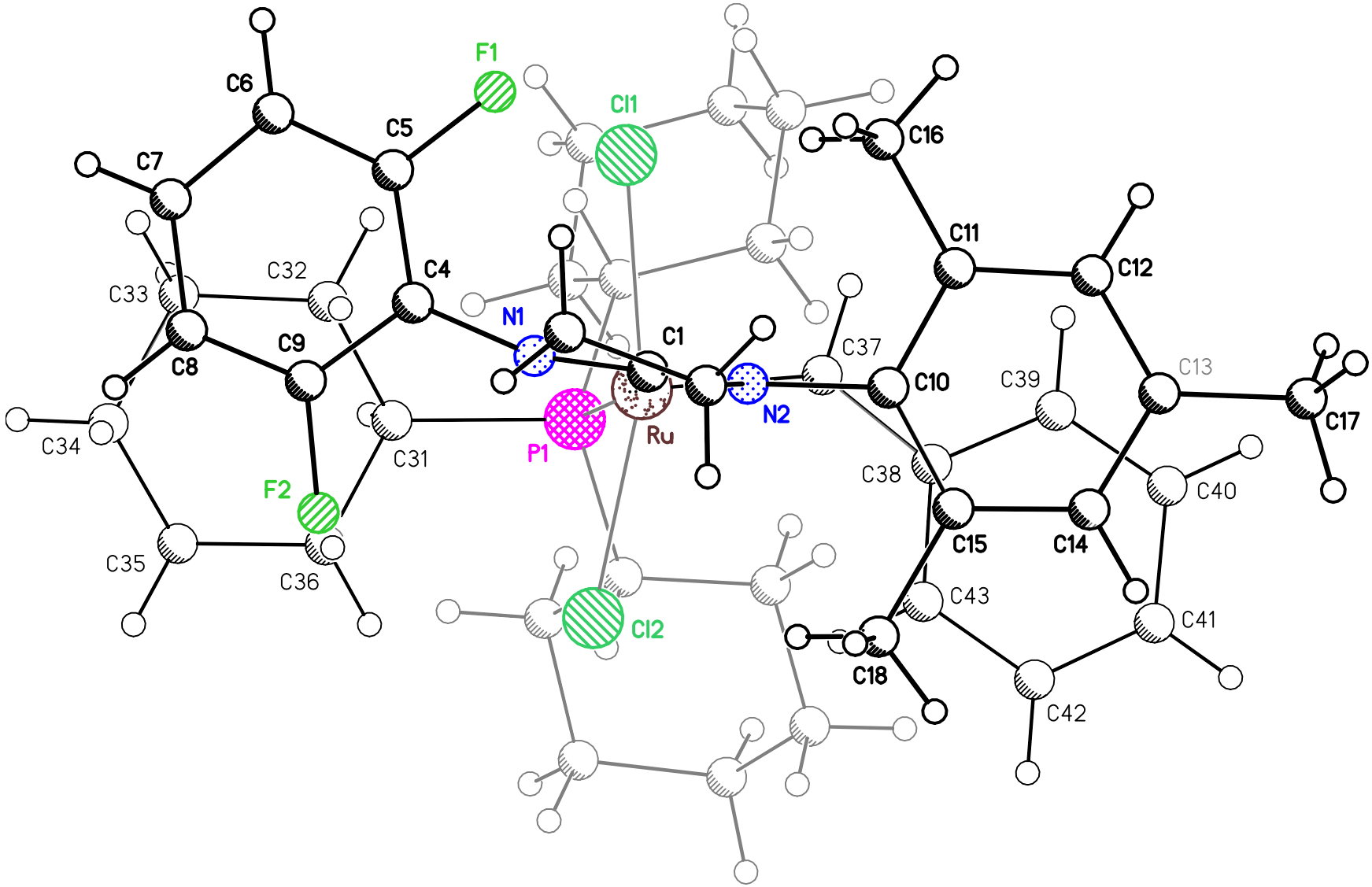
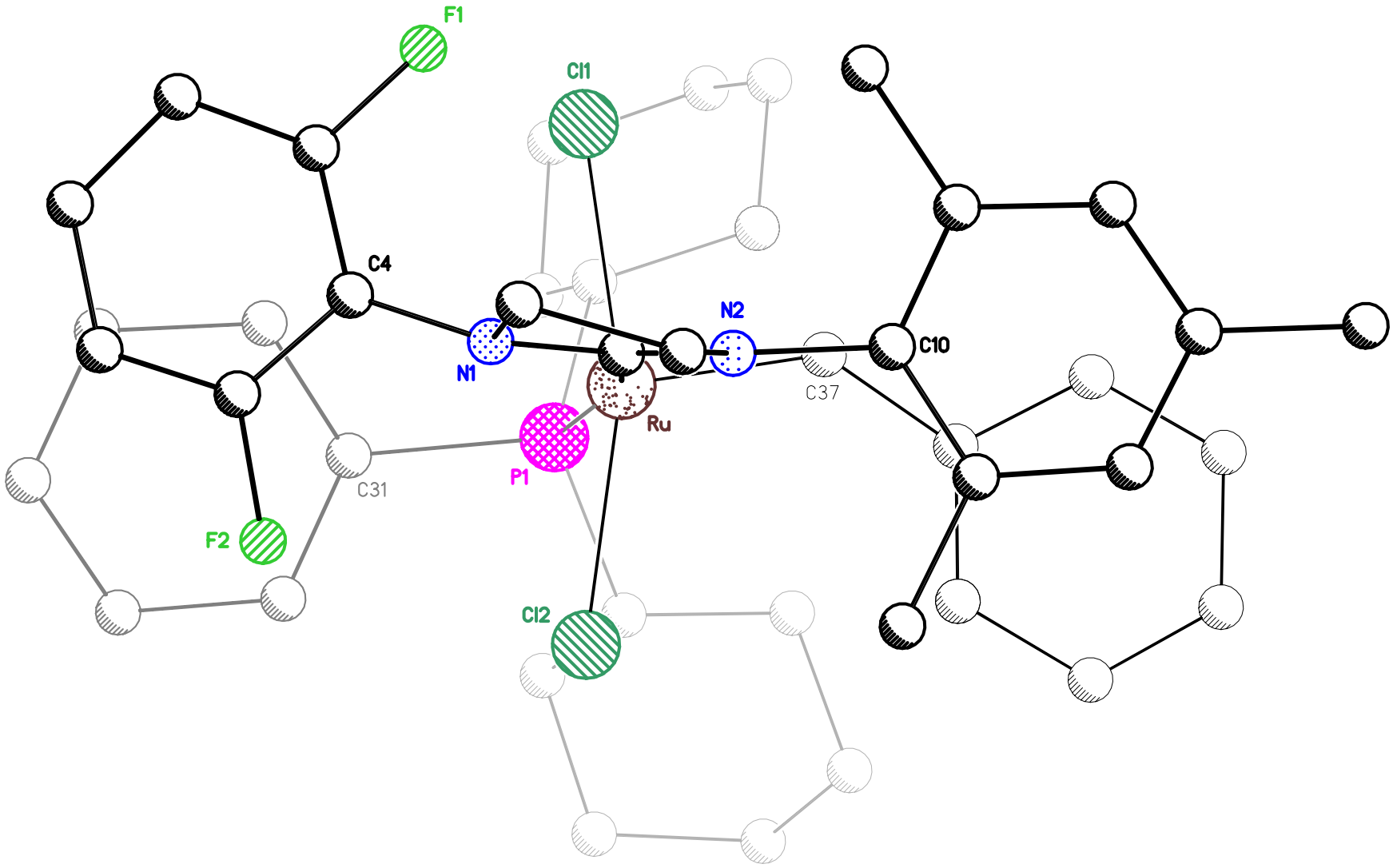
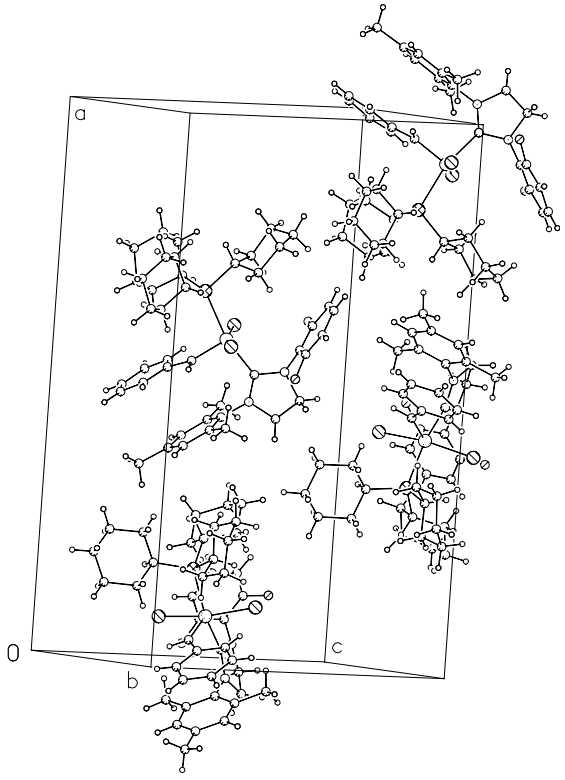
C17
C15
C8
C18
C14
F2
Cl1
Ru
C38
C37
C39
Cl2
C33
C32
C40
C34
C43
C31
C19
C21
P1
C42
C41
C20
C36
C35
C25
C24
C26
C23
C22
C30
C27
C29
C28


F1
C6
C5
C7
Cl1
C16
C11
C12
C32
C4
C33
N1
C1
C37
C9
C8
C10
C39
C13
C17
C34
P1
Ru
N2
C31
C38
C40
F2
C15
C14
C35
C36
C43
C41
Cl2
C18
C42


F1
Cl1
C4
N2
C10
N1
C37
Ru
P1
C31
F2
Cl2


a
0
b
c

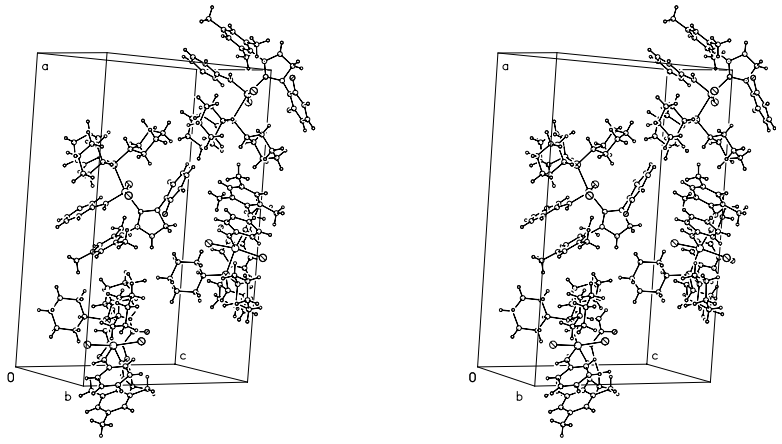

a
c
0
b
a
c
0
b

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for CCDC 621770. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru	789(1)	2430(1)	4835(1)	20(1)
P(1)	1642(1)	2818(1)	4159(1)	18(1)
Cl(1)	709(1)	291(1)	4127(1)	29(1)
Cl(2)	1021(1)	4202(1)	5792(1)	25(1)
F(1)	206(2)	-1430(3)	5681(2)	73(1)
F(2)	1193(1)	1648(3)	7252(2)	55(1)
N(1)	275(1)	1106(3)	6342(2)	29(1)
N(2)	-317(1)	2327(3)	5700(2)	31(1)
C(1)	186(2)	1913(4)	5654(2)	24(1)
C(2)	-226(2)	767(5)	6787(3)	50(1)
C(3)	-594(2)	1888(6)	6467(3)	50(1)
C(4)	699(2)	151(4)	6420(2)	28(1)
C(5)	658(2)	-1126(4)	6100(3)	46(1)
C(6)	1039(3)	-2126(5)	6215(4)	77(2)
C(7)	1479(3)	-1771(8)	6687(4)	87(3)
C(8)	1524(2)	-529(7)	7025(3)	61(2)
C(9)	1141(2)	414(5)	6894(2)	36(1)
C(10)	-627(2)	3065(4)	5093(2)	29(1)
C(11)	-854(2)	2334(4)	4437(3)	35(1)
C(12)	-1167(2)	3076(4)	3873(3)	35(1)
C(13)	-1242(2)	4458(4)	3944(3)	36(1)
C(14)	-1024(2)	5132(4)	4629(3)	34(1)
C(15)	-711(2)	4454(4)	5206(3)	32(1)
C(16)	-778(2)	831(5)	4353(3)	43(1)
C(17)	-1561(2)	5242(5)	3307(3)	51(1)
C(18)	-464(2)	5214(5)	5934(3)	39(1)
C(19)	1712(1)	1965(4)	3128(2)	21(1)
C(20)	1287(2)	2331(5)	2485(2)	37(1)
C(21)	1312(2)	1353(5)	1749(3)	45(1)
C(22)	1852(2)	1294(5)	1351(3)	39(1)
C(23)	2262(2)	966(5)	1979(3)	45(1)
C(24)	2250(2)	2004(5)	2697(3)	41(1)
C(25)	1868(1)	4612(3)	4076(2)	22(1)
C(26)	1566(2)	5439(4)	3416(3)	41(1)
C(27)	1677(2)	6960(4)	3511(3)	44(1)
C(28)	2268(2)	7244(4)	3454(3)	30(1)
C(29)	2596(2)	6359(4)	4039(3)	32(1)
C(30)	2463(1)	4853(4)	3935(2)	26(1)
C(31)	2177(1)	2000(3)	4768(3)	19(1)
C(32)	2060(1)	499(3)	4965(2)	27(1)
C(33)	2553(2)	-192(4)	5342(3)	35(1)
C(34)	2766(2)	582(4)	6092(3)	36(1)
C(35)	2832(2)	2091(4)	5935(3)	32(1)
C(36)	2314(2)	2713(4)	5588(2)	27(1)
C(37)	370(2)	3196(4)	4011(2)	28(1)
C(38)	207(2)	4550(4)	3767(2)	29(1)
C(39)	-93(2)	4701(5)	3042(3)	37(1)
C(40)	-297(2)	5924(5)	2792(3)	46(1)

C(41)	-188(2)	7072(5)	3284(3)	55(1)
C(42)	113(2)	6975(5)	3988(3)	51(1)
C(43)	313(2)	5728(4)	4234(3)	35(1)

Table 3. Selected bond lengths [Å] and angles [°] for CCDC 621770.

Ru-C(37)	1.851(4)	C(37)-Ru-C(1)	97.60(16)
Ru-C(1)	2.071(4)	C(37)-Ru-Cl(2)	107.61(12)
Ru-Cl(2)	2.3898(9)	C(1)-Ru-Cl(2)	87.16(11)
Ru-Cl(1)	2.3931(9)	C(37)-Ru-Cl(1)	88.21(12)
Ru-P(1)	2.4379(9)	C(1)-Ru-Cl(1)	91.36(11)
		Cl(2)-Ru-Cl(1)	164.17(3)
		C(37)-Ru-P(1)	97.05(12)
		C(1)-Ru-P(1)	165.32(11)
		Cl(2)-Ru-P(1)	87.52(3)
		Cl(1)-Ru-P(1)	90.03(3)

Table 4. Bond lengths [Å] and angles [°] for CCDC 621770.

Ru-C(37)	1.851(4)	C(38)-C(39)	1.395(6)
Ru-C(1)	2.071(4)	C(38)-C(43)	1.402(6)
Ru-Cl(2)	2.3898(9)	C(39)-C(40)	1.364(6)
Ru-Cl(1)	2.3931(9)	C(40)-C(41)	1.401(7)
Ru-P(1)	2.4379(9)	C(41)-C(42)	1.363(7)
P(1)-C(31)	1.848(3)	C(42)-C(43)	1.380(6)
P(1)-C(25)	1.853(3)		
P(1)-C(19)	1.860(4)	C(37)-Ru-C(1)	97.60(16)
F(1)-C(5)	1.356(6)	C(37)-Ru-Cl(2)	107.61(12)
F(2)-C(9)	1.345(6)	C(1)-Ru-Cl(2)	87.16(11)
N(1)-C(1)	1.376(5)	C(37)-Ru-Cl(1)	88.21(12)
N(1)-C(4)	1.425(5)	C(1)-Ru-Cl(1)	91.36(11)
N(1)-C(2)	1.488(5)	Cl(2)-Ru-Cl(1)	164.17(3)
N(2)-C(1)	1.332(5)	C(37)-Ru-P(1)	97.05(12)
N(2)-C(10)	1.442(5)	C(1)-Ru-P(1)	165.32(11)
N(2)-C(3)	1.479(5)	Cl(2)-Ru-P(1)	87.52(3)
C(2)-C(3)	1.527(6)	Cl(1)-Ru-P(1)	90.03(3)
C(4)-C(5)	1.357(6)	C(31)-P(1)-C(25)	102.99(15)
C(4)-C(9)	1.373(6)	C(31)-P(1)-C(19)	101.86(17)
C(5)-C(6)	1.385(8)	C(25)-P(1)-C(19)	109.52(17)
C(6)-C(7)	1.389(10)	C(31)-P(1)-Ru	109.91(12)
C(7)-C(8)	1.337(10)	C(25)-P(1)-Ru	116.80(11)
C(8)-C(9)	1.354(7)	C(19)-P(1)-Ru	114.12(11)
C(10)-C(15)	1.391(6)	C(1)-N(1)-C(4)	124.8(3)
C(10)-C(11)	1.396(6)	C(1)-N(1)-C(2)	111.9(3)
C(11)-C(12)	1.403(6)	C(4)-N(1)-C(2)	116.6(3)
C(11)-C(16)	1.492(6)	C(1)-N(2)-C(10)	129.1(3)
C(12)-C(13)	1.372(6)	C(1)-N(2)-C(3)	114.0(3)
C(13)-C(14)	1.395(6)	C(10)-N(2)-C(3)	116.8(3)
C(13)-C(17)	1.511(6)	N(2)-C(1)-N(1)	106.6(3)
C(14)-C(15)	1.385(6)	N(2)-C(1)-Ru	131.2(3)
C(15)-C(18)	1.517(6)	N(1)-C(1)-Ru	121.9(3)
C(19)-C(24)	1.523(5)	N(1)-C(2)-C(3)	101.2(3)
C(19)-C(20)	1.529(5)	N(2)-C(3)-C(2)	101.6(3)
C(20)-C(21)	1.522(6)	C(5)-C(4)-C(9)	116.4(4)
C(21)-C(22)	1.505(6)	C(5)-C(4)-N(1)	121.0(4)
C(22)-C(23)	1.477(7)	C(9)-C(4)-N(1)	122.2(4)
C(23)-C(24)	1.537(6)	F(1)-C(5)-C(4)	117.0(4)
C(25)-C(30)	1.535(5)	F(1)-C(5)-C(6)	119.6(5)
C(25)-C(26)	1.536(6)	C(4)-C(5)-C(6)	123.4(5)
C(26)-C(27)	1.525(6)	C(7)-C(6)-C(5)	116.7(5)
C(27)-C(28)	1.517(6)	C(8)-C(7)-C(6)	121.1(5)
C(28)-C(29)	1.522(5)	C(7)-C(8)-C(9)	119.9(6)
C(29)-C(30)	1.523(5)	F(2)-C(9)-C(8)	118.5(5)
C(31)-C(36)	1.528(5)	F(2)-C(9)-C(4)	119.0(4)
C(31)-C(32)	1.534(4)	C(8)-C(9)-C(4)	122.5(5)
C(32)-C(33)	1.539(5)	C(15)-C(10)-C(11)	122.6(4)
C(33)-C(34)	1.519(6)	C(15)-C(10)-N(2)	119.1(4)
C(34)-C(35)	1.510(6)	C(11)-C(10)-N(2)	118.3(4)
C(35)-C(36)	1.544(5)	C(10)-C(11)-C(12)	116.8(4)
C(37)-C(38)	1.443(6)	C(10)-C(11)-C(16)	121.5(4)

C(12)-C(11)-C(16)	121.8(4)
C(13)-C(12)-C(11)	122.4(4)
C(12)-C(13)-C(14)	118.6(4)
C(12)-C(13)-C(17)	121.3(4)
C(14)-C(13)-C(17)	120.1(4)
C(15)-C(14)-C(13)	121.6(4)
C(10)-C(15)-C(14)	118.0(4)
C(10)-C(15)-C(18)	121.3(4)
C(14)-C(15)-C(18)	120.7(4)
C(24)-C(19)-C(20)	108.3(3)
C(24)-C(19)-P(1)	118.4(3)
C(20)-C(19)-P(1)	115.3(3)
C(21)-C(20)-C(19)	110.2(3)
C(22)-C(21)-C(20)	113.0(4)
C(23)-C(22)-C(21)	110.6(4)
C(22)-C(23)-C(24)	110.7(4)
C(19)-C(24)-C(23)	109.9(3)
C(30)-C(25)-C(26)	107.6(3)
C(30)-C(25)-P(1)	117.2(2)
C(26)-C(25)-P(1)	113.4(3)
C(27)-C(26)-C(25)	110.8(4)
C(28)-C(27)-C(26)	110.8(4)
C(27)-C(28)-C(29)	113.1(3)
C(30)-C(29)-C(28)	111.4(3)
C(29)-C(30)-C(25)	110.4(3)
C(36)-C(31)-C(32)	107.8(3)
C(36)-C(31)-P(1)	114.9(2)
C(32)-C(31)-P(1)	112.6(2)
C(31)-C(32)-C(33)	110.4(3)
C(34)-C(33)-C(32)	112.1(3)
C(35)-C(34)-C(33)	113.4(3)
C(34)-C(35)-C(36)	110.7(3)
C(31)-C(36)-C(35)	108.7(3)
C(38)-C(37)-Ru	136.8(3)
C(39)-C(38)-C(43)	117.4(4)
C(39)-C(38)-C(37)	118.6(4)
C(43)-C(38)-C(37)	124.0(4)
C(40)-C(39)-C(38)	122.8(4)
C(39)-C(40)-C(41)	117.8(4)
C(42)-C(41)-C(40)	121.3(4)
C(41)-C(42)-C(43)	120.1(5)
C(42)-C(43)-C(38)	120.6(4)

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for CCDC 621770. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru	176(1)	165(1)	252(1)	29(1)	58(1)	9(1)
P(1)	201(4)	127(4)	223(4)	14(3)	52(4)	0(3)
Cl(1)	255(4)	207(4)	399(5)	-27(4)	53(4)	-33(3)
Cl(2)	277(4)	231(4)	252(4)	-17(3)	68(4)	9(3)
F(1)	1070(30)	432(18)	690(20)	17(16)	-130(20)	-453(17)
F(2)	566(18)	750(20)	346(15)	-76(14)	-47(14)	-206(16)
N(1)	190(15)	337(19)	343(18)	103(15)	90(13)	-2(13)
N(2)	211(14)	364(19)	341(19)	155(15)	50(13)	64(14)
C(1)	292(19)	174(17)	270(20)	28(14)	32(16)	-17(15)
C(2)	220(20)	760(40)	520(30)	380(30)	140(20)	70(20)
C(3)	280(20)	700(30)	520(30)	370(30)	150(20)	120(20)
C(4)	340(20)	260(20)	241(19)	82(14)	70(16)	1(16)
C(5)	750(40)	270(20)	360(30)	43(18)	20(20)	-50(20)
C(6)	1560(70)	260(30)	480(40)	130(20)	270(40)	320(30)
C(7)	920(50)	1200(60)	490(40)	550(40)	350(30)	810(50)
C(8)	410(30)	1130(50)	300(30)	250(30)	80(20)	260(30)
C(9)	290(20)	610(30)	175(19)	96(18)	65(16)	-60(20)
C(10)	195(16)	350(20)	320(20)	95(15)	43(15)	66(16)
C(11)	201(18)	340(20)	510(20)	76(19)	37(16)	14(17)
C(12)	248(19)	430(20)	380(20)	-52(18)	-12(18)	-2(18)
C(13)	216(18)	450(30)	410(30)	47(19)	7(17)	80(17)
C(14)	285(19)	350(20)	390(30)	33(17)	51(16)	116(17)
C(15)	270(20)	390(20)	280(20)	5(17)	38(17)	51(18)
C(16)	330(20)	410(30)	560(30)	30(20)	-20(20)	-100(20)
C(17)	450(30)	540(30)	530(30)	40(20)	-110(20)	160(20)
C(18)	360(20)	430(30)	390(30)	19(19)	58(19)	110(20)
C(19)	218(16)	228(17)	197(17)	-16(13)	5(14)	-51(14)
C(20)	390(20)	450(30)	260(20)	10(19)	27(17)	140(20)
C(21)	470(30)	660(30)	230(20)	-30(20)	-10(20)	30(20)
C(22)	500(30)	320(20)	340(20)	-122(18)	130(20)	-75(19)
C(23)	380(20)	560(30)	410(30)	-300(20)	50(20)	60(20)
C(24)	280(20)	590(30)	370(30)	-220(20)	21(18)	-50(20)
C(25)	207(15)	147(16)	310(20)	18(14)	64(15)	-46(12)
C(26)	350(20)	260(20)	610(30)	130(20)	-30(20)	-75(17)
C(27)	380(20)	220(20)	720(30)	170(20)	30(20)	-17(18)
C(28)	350(20)	200(20)	340(20)	33(15)	34(17)	-86(15)
C(29)	300(20)	290(20)	350(20)	45(17)	-31(18)	-147(16)
C(30)	225(17)	227(19)	320(20)	49(15)	16(16)	-51(14)
C(31)	131(12)	195(14)	239(18)	21(17)	-40(16)	17(10)
C(32)	297(17)	214(17)	290(20)	41(15)	2(16)	22(14)
C(33)	380(20)	260(20)	410(30)	39(18)	-90(20)	141(18)
C(34)	330(20)	420(30)	320(20)	82(18)	-63(18)	89(18)
C(35)	271(19)	430(20)	250(20)	14(16)	-36(16)	-54(17)
C(36)	309(18)	230(20)	270(20)	14(15)	48(15)	36(15)
C(37)	279(19)	360(20)	200(20)	-56(16)	26(16)	-46(16)
C(38)	207(18)	390(20)	270(20)	23(17)	35(15)	29(16)
C(39)	350(20)	480(30)	280(20)	-19(19)	44(18)	-30(20)

C(40)	460(30)	620(30)	300(20)	100(20)	-110(20)	90(20)
C(41)	800(40)	410(30)	450(30)	110(20)	-100(30)	170(30)
C(42)	740(40)	310(20)	480(30)	60(20)	-120(30)	-10(20)
C(43)	460(20)	300(20)	270(20)	39(17)	-49(18)	-4(18)

[$RuCl_2$ (1-(2,6-difluorophenyl)-3-mesityl-dihydroimidazol-ylidene) (=CH-*o*-*i*PrO-Ph)] (6)

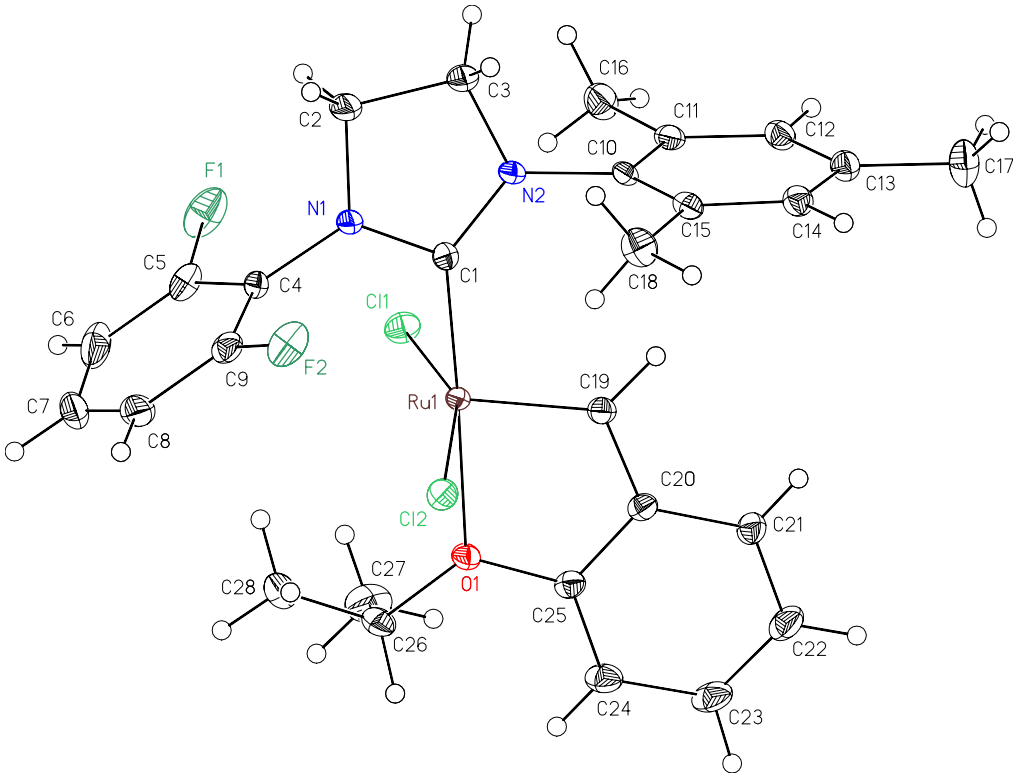


Table 1. Crystal data and structure refinement for CCDC 612854.

Empirical formula	$C_{28}H_{30}F_2N_2OCl_2Ru$
Formula weight	620.51
Crystallization Solvent	Toluene
Crystal Habit	Blade
Crystal size	0.27 x 0.22 x 0.15 mm^3
Crystal color	Trichroic - Brown/olive/bright green

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 24143 reflections used in lattice determination	2.39 to 43.26°
Unit cell dimensions	a = 17.0577(5) Å b = 10.1643(3) Å β= 113.5310(10)° c = 17.1021(5) Å
Volume	2718.58(14) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.516 Mg/m^3
F(000)	1264
Data collection program	Bruker SMART v5.630
θ range for data collection	2.39 to 44.11°
Completeness to θ = 44.11°	88.5 %
Index ranges	$-30 \le h \le 33$, $-18 \le k \le 18$, $-31 \le l \le 31$
Data collection scan type	ω scans at 8 ϕ settings
Data reduction program	Bruker SAINT v6.45A
Reflections collected	64388
Independent reflections	18912 [R_{int}= 0.0748]
Absorption coefficient	0.811 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.8880 and 0.8108

Table 1 (cont.)

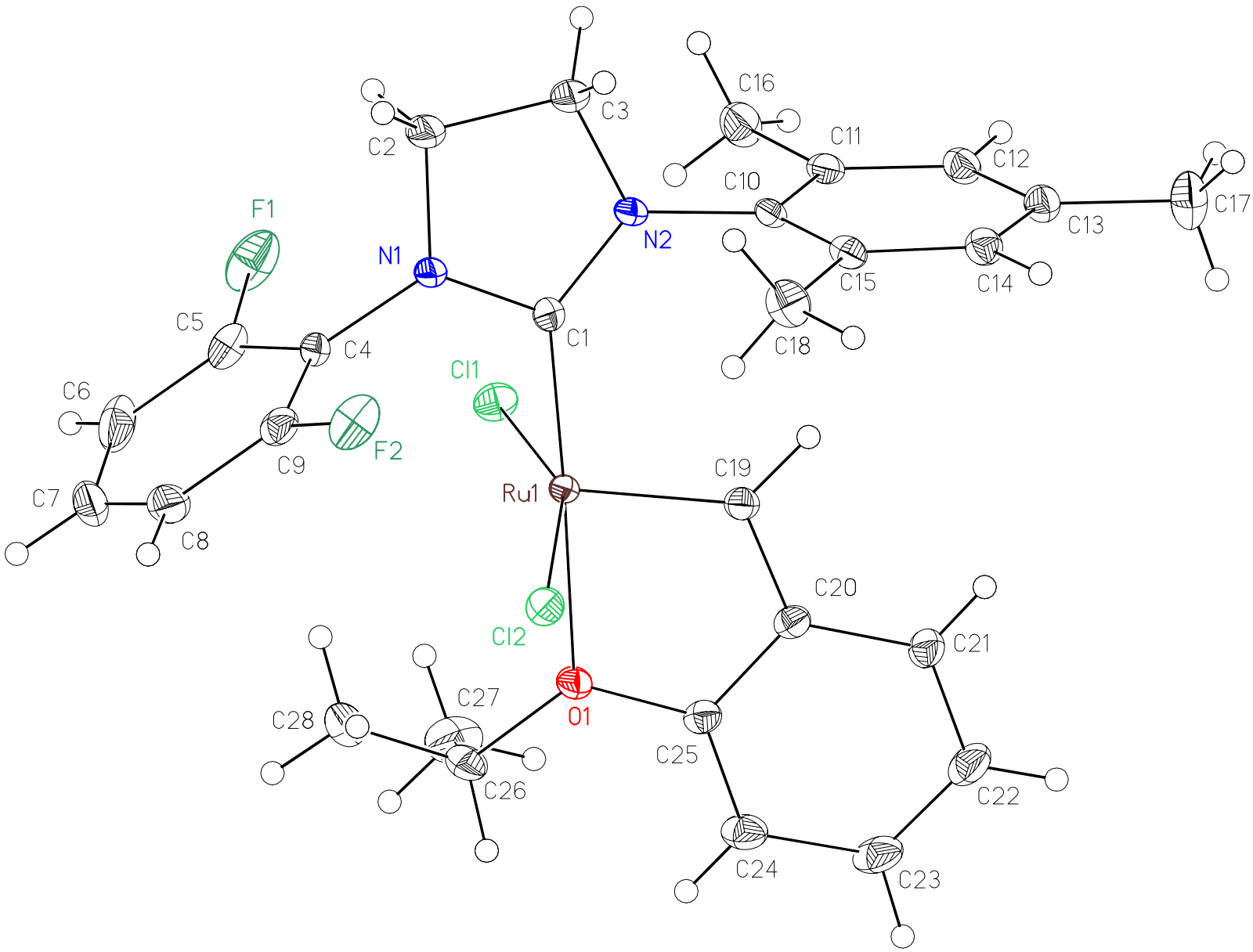
Structure solution and Refinement

Structure solution program	Bruker XS v6.12
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	Bruker XL v6.12
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	18912 / 0 / 445
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.145
Final R indices [$I>2\sigma(I)$, 12464 reflections]	R1 = 0.0364, *w*R2 = 0.0662
R indices (all data)	R1 = 0.0702, *w*R2 = 0.0718
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.002
Average shift/error	0.000
Largest diff. peak and hole	1.213 and -0.739 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C16
C3
C2
C11
C12
C10
C17
F1
N2
C13
N1
C15
C14
C5
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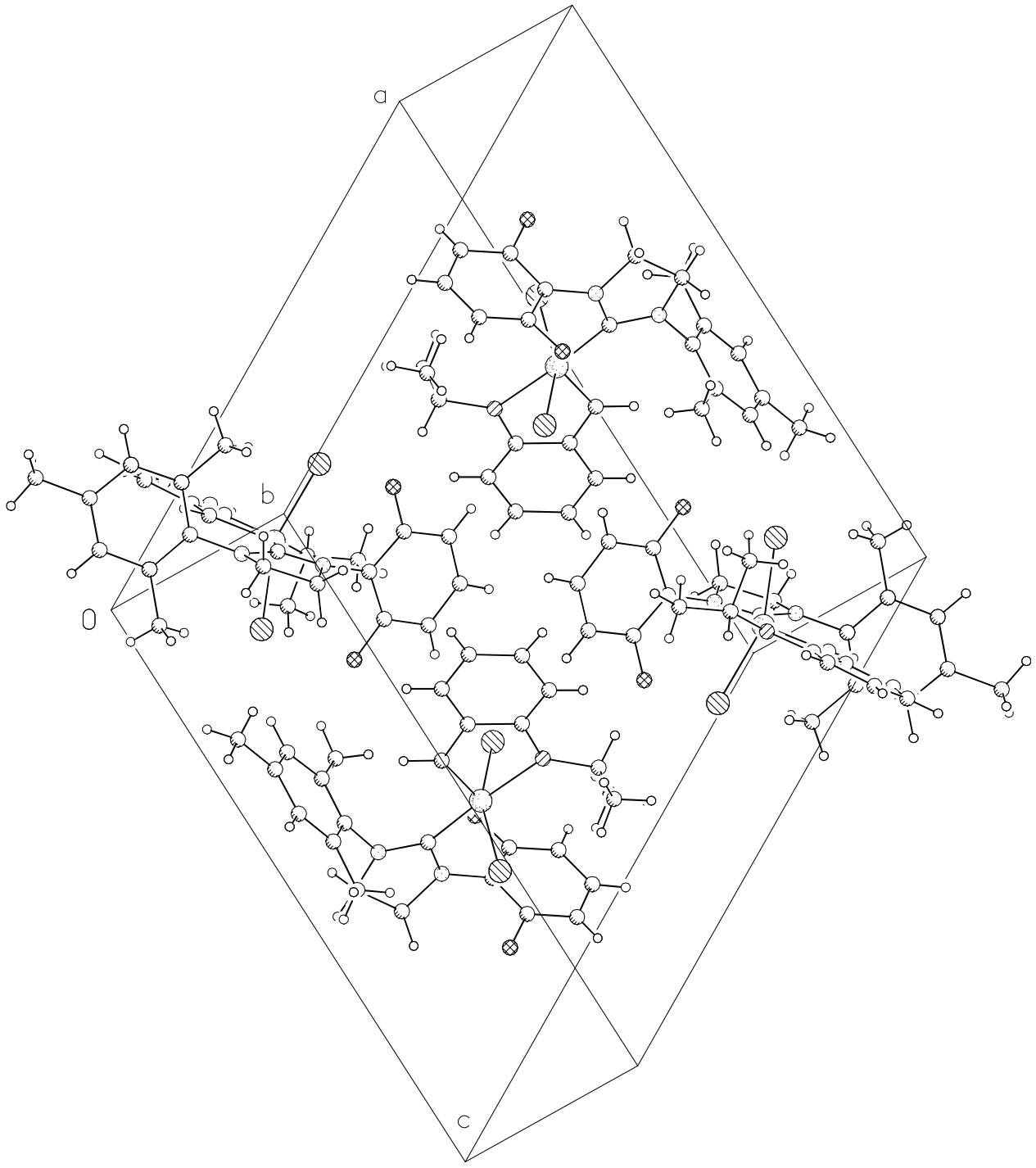
C18
C4
Cl1
C6
F2
C9
C19
C7
Ru1
C8
C20
Cl2
C21
C27
O1
C28
C25
C22
C26
C24
C23


a
b
c
O

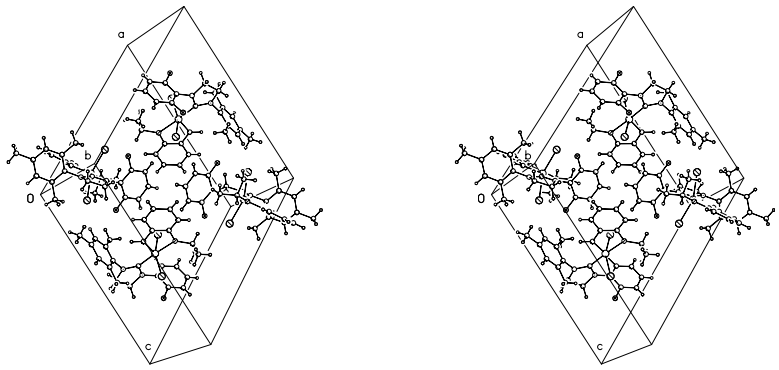

a
b
0
c
a
b
0
c

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for CCDC 612854. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	2741(1)	1641(1)	1568(1)	10(1)
Cl(1)	1971(1)	724(1)	2293(1)	18(1)
Cl(2)	3919(1)	2604(1)	1418(1)	16(1)
F(1)	2248(1)	3116(1)	3517(1)	32(1)
F(2)	3869(1)	5257(1)	2250(1)	25(1)
O(1)	3467(1)	-261(1)	1802(1)	14(1)
N(1)	2315(1)	4190(1)	2052(1)	17(1)
N(2)	1313(1)	3672(1)	829(1)	15(1)
C(1)	2072(1)	3269(1)	1420(1)	13(1)
C(2)	1656(1)	5182(2)	1952(1)	26(1)
C(3)	1042(1)	4965(2)	1031(1)	23(1)
C(4)	3049(1)	4063(1)	2825(1)	13(1)
C(5)	3018(1)	3486(1)	3552(1)	19(1)
C(6)	3736(1)	3322(2)	4299(1)	28(1)
C(7)	4504(1)	3790(2)	4332(1)	31(1)
C(8)	4563(1)	4455(2)	3650(1)	25(1)
C(9)	3835(1)	4583(1)	2911(1)	17(1)
C(10)	870(1)	3154(1)	-15(1)	13(1)
C(11)	171(1)	2305(1)	-178(1)	14(1)
C(12)	-271(1)	1859(1)	-1012(1)	16(1)
C(13)	-39(1)	2260(1)	-1672(1)	16(1)
C(14)	657(1)	3107(1)	-1486(1)	16(1)
C(15)	1121(1)	3564(1)	-662(1)	14(1)
C(16)	-101(1)	1892(2)	520(1)	22(1)
C(17)	-519(1)	1769(2)	-2569(1)	27(1)
C(18)	1888(1)	4440(2)	-474(1)	21(1)
C(19)	2241(1)	894(1)	507(1)	14(1)
C(20)	2563(1)	-364(1)	367(1)	13(1)
C(21)	2276(1)	-979(1)	-432(1)	17(1)
C(22)	2617(1)	-2177(1)	-532(1)	22(1)
C(23)	3245(1)	-2773(1)	172(1)	23(1)
C(24)	3544(1)	-2193(1)	973(1)	19(1)
C(25)	3210(1)	-990(1)	1063(1)	14(1)
C(26)	4066(1)	-824(1)	2619(1)	19(1)
C(27)	3608(1)	-1823(2)	2940(1)	28(1)
C(28)	4416(1)	319(2)	3221(1)	26(1)

Table 3. Selected bond lengths [Å] and angles [°] for CCDC 612854.

Ru(1)-C(19)	1.8337(12)	C(19)-Ru(1)-C(1)	101.74(5)
Ru(1)-C(1)	1.9688(12)	C(19)-Ru(1)-O(1)	79.94(4)
Ru(1)-O(1)	2.2441(8)	C(1)-Ru(1)-O(1)	176.05(4)
Ru(1)-Cl(1)	2.3303(3)	C(19)-Ru(1)-Cl(1)	102.81(4)
Ru(1)-Cl(2)	2.3396(3)	C(1)-Ru(1)-Cl(1)	89.08(4)
		O(1)-Ru(1)-Cl(1)	87.06(2)
		C(19)-Ru(1)-Cl(2)	98.37(4)
		C(1)-Ru(1)-Cl(2)	96.52(4)
		O(1)-Ru(1)-Cl(2)	86.72(2)
		Cl(1)-Ru(1)-Cl(2)	156.505(12)

Table 4. Bond lengths [Å] and angles [°] for CCDC 612854.

Ru(1)-C(19)	1.8337(12)	C(20)-C(21)	1.4023(17)
Ru(1)-C(1)	1.9688(12)	C(20)-C(25)	1.4109(17)
Ru(1)-O(1)	2.2441(8)	C(21)-C(22)	1.3899(19)
Ru(1)-Cl(1)	2.3303(3)	C(21)-H(21)	0.918(17)
Ru(1)-Cl(2)	2.3396(3)	C(22)-C(23)	1.391(2)
F(1)-C(5)	1.3440(16)	C(22)-H(22)	0.905(16)
F(2)-C(9)	1.3419(15)	C(23)-C(24)	1.387(2)
O(1)-C(25)	1.3775(15)	C(23)-H(23)	0.955(17)
O(1)-C(26)	1.4775(15)	C(24)-C(25)	1.3833(18)
N(1)-C(1)	1.3637(15)	C(24)-H(24)	0.892(16)
N(1)-C(4)	1.4184(15)	C(26)-C(28)	1.508(2)
N(1)-C(2)	1.4685(16)	C(26)-C(27)	1.511(2)
N(2)-C(1)	1.3489(15)	C(26)-H(26)	0.941(17)
N(2)-C(10)	1.4365(16)	C(27)-H(27A)	0.93(2)
N(2)-C(3)	1.4782(17)	C(27)-H(27B)	0.97(2)
C(2)-C(3)	1.520(2)	C(27)-H(27C)	0.96(2)
C(2)-H(2A)	0.927(18)	C(28)-H(28A)	0.985(17)
C(2)-H(2B)	1.018(19)	C(28)-H(28B)	0.95(2)
C(3)-H(3A)	0.947(18)	C(28)-H(28C)	0.960(18)
C(3)-H(3B)	0.965(18)		
C(4)-C(5)	1.3950(18)	C(19)-Ru(1)-C(1)	101.74(5)
C(4)-C(9)	1.3935(18)	C(19)-Ru(1)-O(1)	79.94(4)
C(5)-C(6)	1.382(2)	C(1)-Ru(1)-O(1)	176.05(4)
C(6)-C(7)	1.374(3)	C(19)-Ru(1)-Cl(1)	102.81(4)
C(6)-H(6)	0.85(2)	C(1)-Ru(1)-Cl(1)	89.08(4)
C(7)-C(8)	1.384(3)	O(1)-Ru(1)-Cl(1)	87.06(2)
C(7)-H(7)	0.92(2)	C(19)-Ru(1)-Cl(2)	98.37(4)
C(8)-C(9)	1.3792(19)	C(1)-Ru(1)-Cl(2)	96.52(4)
C(8)-H(8)	0.93(2)	O(1)-Ru(1)-Cl(2)	86.72(2)
C(10)-C(15)	1.3984(17)	Cl(1)-Ru(1)-Cl(2)	156.505(12)
C(10)-C(11)	1.4069(17)	C(25)-O(1)-C(26)	120.40(9)
C(11)-C(12)	1.3960(18)	C(25)-O(1)-Ru(1)	110.41(7)
C(11)-C(16)	1.5020(19)	C(26)-O(1)-Ru(1)	128.80(7)
C(12)-C(13)	1.3978(18)	C(1)-N(1)-C(4)	123.52(10)
C(12)-H(12)	0.957(16)	C(1)-N(1)-C(2)	113.77(10)
C(13)-C(14)	1.3961(18)	C(4)-N(1)-C(2)	121.45(10)
C(13)-C(17)	1.5058(19)	C(1)-N(2)-C(10)	127.11(10)
C(14)-C(15)	1.3922(18)	C(1)-N(2)-C(3)	113.03(10)
C(14)-H(14)	0.962(16)	C(10)-N(2)-C(3)	118.20(10)
C(15)-C(18)	1.5071(18)	N(2)-C(1)-N(1)	106.39(10)
C(16)-H(16A)	0.96(2)	N(2)-C(1)-Ru(1)	133.30(9)
C(16)-H(16B)	0.87(2)	N(1)-C(1)-Ru(1)	119.83(8)
C(16)-H(16C)	0.92(2)	N(1)-C(2)-C(3)	101.49(10)
C(17)-H(17A)	0.97(2)	N(1)-C(2)-H(2A)	111.8(11)
C(17)-H(17B)	0.98(2)	C(3)-C(2)-H(2A)	114.6(11)
C(17)-H(17C)	0.86(2)	N(1)-C(2)-H(2B)	107.1(10)
C(18)-H(18A)	0.94(2)	C(3)-C(2)-H(2B)	114.1(11)
C(18)-H(18B)	0.87(2)	H(2A)-C(2)-H(2B)	107.6(14)
C(18)-H(18C)	0.97(2)	N(2)-C(3)-C(2)	102.78(11)
C(19)-C(20)	1.4481(17)	N(2)-C(3)-H(3A)	113.9(11)
C(19)-H(19)	0.997(16)	C(2)-C(3)-H(3A)	109.1(10)

N(2)-C(3)-H(3B)	110.8(11)
C(2)-C(3)-H(3B)	111.9(11)
H(3A)-C(3)-H(3B)	108.4(15)
C(5)-C(4)-C(9)	116.32(12)
C(5)-C(4)-N(1)	122.32(12)
C(9)-C(4)-N(1)	121.25(12)
F(1)-C(5)-C(6)	119.82(13)
F(1)-C(5)-C(4)	117.50(12)
C(6)-C(5)-C(4)	122.64(13)
C(7)-C(6)-C(5)	118.32(14)
C(7)-C(6)-H(6)	122.3(14)
C(5)-C(6)-H(6)	119.3(14)
C(6)-C(7)-C(8)	121.51(14)
C(6)-C(7)-H(7)	115.8(14)
C(8)-C(7)-H(7)	122.7(14)
C(9)-C(8)-C(7)	118.52(14)
C(9)-C(8)-H(8)	119.8(13)
C(7)-C(8)-H(8)	121.7(13)
F(2)-C(9)-C(8)	119.67(13)
F(2)-C(9)-C(4)	117.92(12)
C(8)-C(9)-C(4)	122.39(13)
C(15)-C(10)-C(11)	121.94(11)
C(15)-C(10)-N(2)	118.81(11)
C(11)-C(10)-N(2)	119.16(11)
C(12)-C(11)-C(10)	118.03(11)
C(12)-C(11)-C(16)	120.59(12)
C(10)-C(11)-C(16)	121.38(12)
C(11)-C(12)-C(13)	121.34(12)
C(11)-C(12)-H(12)	118.7(9)
C(13)-C(12)-H(12)	119.8(9)
C(14)-C(13)-C(12)	118.90(12)
C(14)-C(13)-C(17)	120.24(12)
C(12)-C(13)-C(17)	120.86(12)
C(15)-C(14)-C(13)	121.68(12)
C(15)-C(14)-H(14)	120.2(10)
C(13)-C(14)-H(14)	118.1(10)
C(14)-C(15)-C(10)	118.10(11)
C(14)-C(15)-C(18)	120.51(12)
C(10)-C(15)-C(18)	121.37(12)
C(11)-C(16)-H(16A)	110.4(12)
C(11)-C(16)-H(16B)	114.8(14)
H(16A)-C(16)-H(16B)	102.2(17)
C(11)-C(16)-H(16C)	111.1(12)
H(16A)-C(16)-H(16C)	112.6(17)
H(16B)-C(16)-H(16C)	105.4(17)
C(13)-C(17)-H(17A)	113.4(13)
C(13)-C(17)-H(17B)	110.5(12)
H(17A)-C(17)-H(17B)	109.3(18)
C(13)-C(17)-H(17C)	108.4(14)
H(17A)-C(17)-H(17C)	106.7(19)
H(17B)-C(17)-H(17C)	108.3(18)
C(15)-C(18)-H(18A)	110.9(12)
C(15)-C(18)-H(18B)	113.2(15)
H(18A)-C(18)-H(18B)	105.5(18)
C(15)-C(18)-H(18C)	113.7(12)
H(18A)-C(18)-H(18C)	111.2(16)
H(18B)-C(18)-H(18C)	101.7(18)
C(20)-C(19)-Ru(1)	118.13(9)
C(20)-C(19)-H(19)	115.8(9)
Ru(1)-C(19)-H(19)	126.1(9)
C(21)-C(20)-C(25)	118.18(11)
C(21)-C(20)-C(19)	123.13(12)
C(25)-C(20)-C(19)	118.67(11)
C(22)-C(21)-C(20)	120.69(13)
C(22)-C(21)-H(21)	121.3(10)
C(20)-C(21)-H(21)	118.0(10)
C(21)-C(22)-C(23)	119.36(13)
C(21)-C(22)-H(22)	119.5(11)
C(23)-C(22)-H(22)	121.1(10)
C(24)-C(23)-C(22)	121.50(12)
C(24)-C(23)-H(23)	116.0(10)
C(22)-C(23)-H(23)	122.5(10)
C(25)-C(24)-C(23)	118.70(13)
C(25)-C(24)-H(24)	120.1(11)
C(23)-C(24)-H(24)	121.1(11)
O(1)-C(25)-C(24)	125.70(12)
O(1)-C(25)-C(20)	112.74(10)
C(24)-C(25)-C(20)	121.54(12)
O(1)-C(26)-C(28)	106.42(11)
O(1)-C(26)-C(27)	109.90(12)
C(28)-C(26)-C(27)	112.97(13)
O(1)-C(26)-H(26)	107.4(10)
C(28)-C(26)-H(26)	109.6(10)
C(27)-C(26)-H(26)	110.3(10)
C(26)-C(27)-H(27A)	112.1(13)
C(26)-C(27)-H(27B)	107.9(12)
H(27A)-C(27)-H(27B)	108.1(17)
C(26)-C(27)-H(27C)	111.2(11)
H(27A)-C(27)-H(27C)	111.3(17)
H(27B)-C(27)-H(27C)	106.0(16)
C(26)-C(28)-H(28A)	113.3(10)
C(26)-C(28)-H(28B)	109.0(12)
H(28A)-C(28)-H(28B)	115.8(16)
C(26)-C(28)-H(28C)	109.5(11)
H(28A)-C(28)-H(28C)	106.9(14)
H(28B)-C(28)-H(28C)	101.5(15

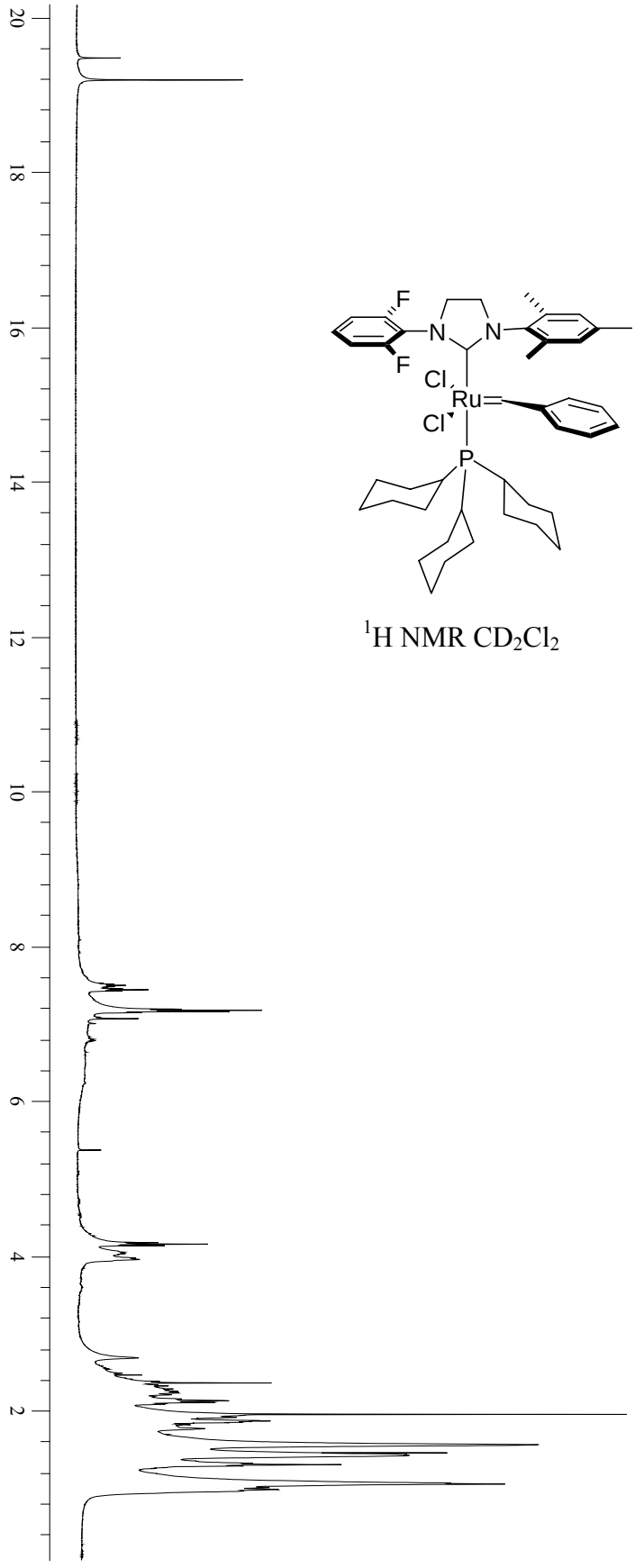
Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for CCDC 612854. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	87(1)	106(1)	107(1)	-10(1)	29(1)	9(1)
Cl(1)	172(1)	188(1)	203(2)	9(1)	111(1)	-1(1)
Cl(2)	129(1)	173(1)	181(1)	-38(1)	68(1)	-35(1)
F(1)	382(5)	322(5)	358(5)	-109(4)	271(5)	-143(4)
F(2)	364(5)	179(4)	286(5)	-27(3)	206(4)	-67(4)
O(1)	144(4)	122(4)	139(4)	3(3)	29(3)	36(3)
N(1)	133(4)	169(5)	146(5)	-52(4)	7(4)	57(4)
N(2)	117(4)	151(5)	142(5)	-30(3)	12(4)	52(4)
C(1)	115(4)	137(5)	122(5)	-16(4)	37(4)	-4(4)
C(2)	188(6)	245(7)	244(7)	-112(6)	-9(5)	95(5)
C(3)	208(6)	218(7)	209(7)	-65(5)	15(5)	108(5)
C(4)	128(5)	132(5)	116(5)	-31(4)	26(4)	8(4)
C(5)	262(6)	165(6)	187(6)	-45(5)	124(5)	-27(5)
C(6)	466(9)	224(7)	131(6)	2(5)	94(6)	59(7)
C(7)	282(8)	309(8)	190(7)	-91(6)	-53(6)	110(6)
C(8)	136(5)	269(7)	289(8)	-132(6)	26(5)	-4(5)
C(9)	180(5)	136(5)	190(6)	-50(4)	79(5)	-14(4)
C(10)	96(4)	131(5)	125(5)	-11(4)	10(4)	27(4)
C(11)	112(5)	155(5)	154(6)	12(4)	50(4)	28(4)
C(12)	120(5)	164(6)	165(6)	-5(4)	38(4)	-7(4)
C(13)	153(5)	153(6)	152(6)	-10(4)	43(4)	2(4)
C(14)	157(5)	169(6)	149(6)	10(4)	59(5)	8(4)
C(15)	116(4)	131(5)	157(5)	9(4)	33(4)	10(4)
C(16)	176(6)	311(8)	172(6)	22(5)	72(5)	-3(5)
C(17)	282(7)	326(9)	167(7)	-51(6)	55(6)	-79(7)
C(18)	183(6)	212(7)	229(7)	-2(5)	72(5)	-57(5)
C(19)	120(5)	128(5)	148(5)	-11(4)	44(4)	6(4)
C(20)	121(5)	127(5)	165(6)	-25(4)	68(4)	-14(4)
C(21)	152(5)	170(6)	170(6)	-50(4)	56(5)	-22(4)
C(22)	214(6)	207(7)	259(7)	-111(5)	115(6)	-32(5)
C(23)	206(6)	142(6)	339(8)	-79(5)	119(6)	3(5)
C(24)	166(5)	138(6)	259(7)	-10(5)	73(5)	21(5)
C(25)	127(5)	121(5)	175(6)	-19(4)	67(4)	-9(4)
C(26)	174(6)	200(6)	172(6)	44(5)	42(5)	69(5)
C(27)	361(8)	229(8)	312(8)	107(6)	190(7)	88(6)
C(28)	223(7)	296(8)	187(7)	-12(6)	14(6)	61(6)

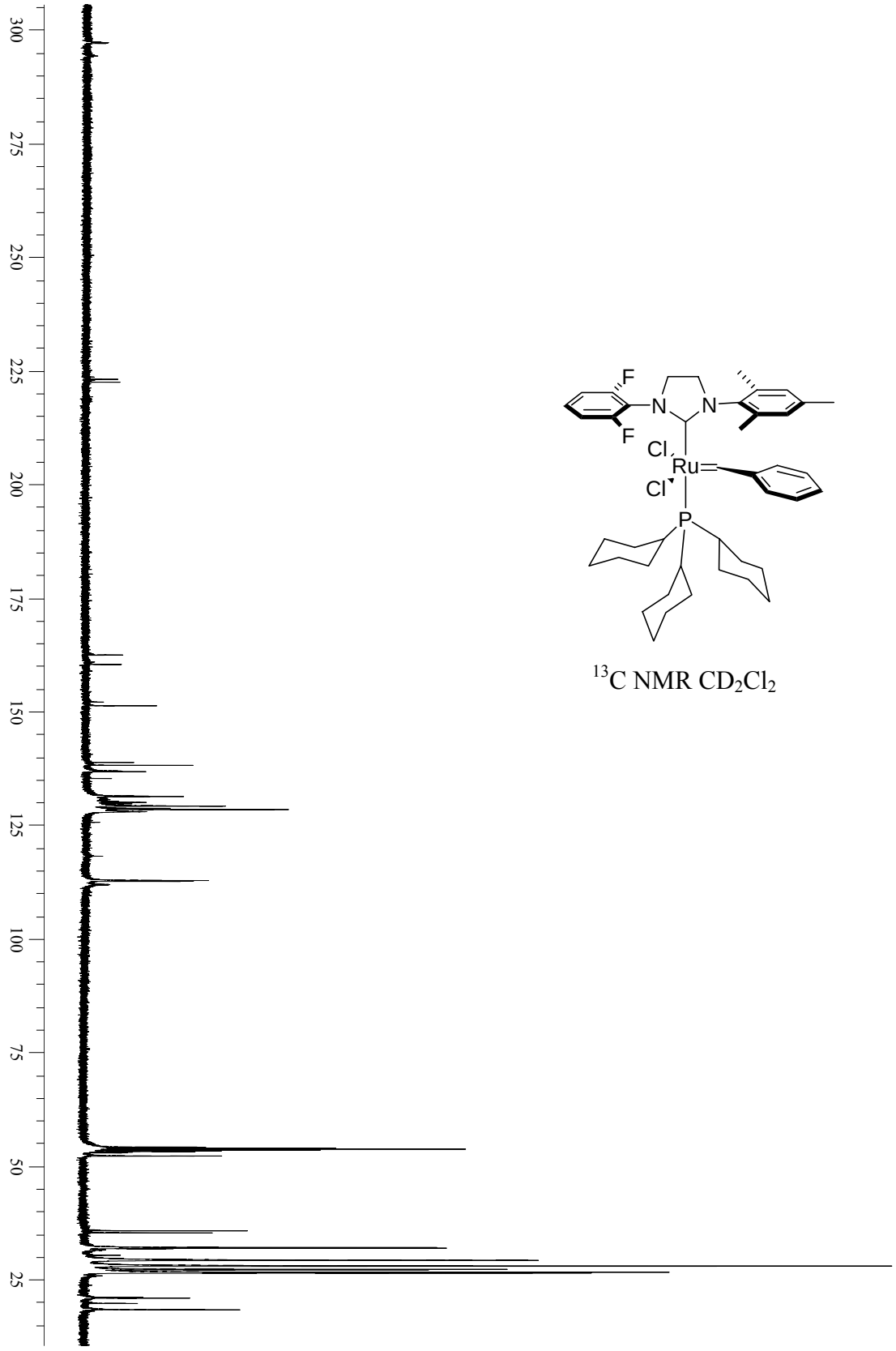
Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for CCDC 612854.

	x	y	z	U_{iso}
H(2A)	1885(11)	6022(18)	2071(11)	25(5)
H(2B)	1404(12)	4968(18)	2386(12)	33(5)
H(3A)	474(11)	4978(17)	997(11)	23(4)
H(3B)	1097(12)	5638(18)	659(11)	30(5)
H(6)	3693(13)	2905(19)	4714(13)	40(6)
H(7)	4966(14)	3660(20)	4836(14)	50(6)
H(8)	5076(13)	4810(20)	3682(13)	46(6)
H(12)	-762(11)	1312(15)	-1135(10)	18(4)
H(14)	815(11)	3364(15)	-1944(10)	18(4)
H(16A)	-351(13)	2620(20)	696(13)	44(6)
H(16B)	313(14)	1660(20)	992(14)	49(6)
H(16C)	-460(13)	1170(20)	357(12)	38(5)
H(17A)	-654(15)	2460(20)	-2997(14)	61(7)
H(17B)	-1047(15)	1330(20)	-2620(13)	50(6)
H(17C)	-201(14)	1210(20)	-2684(13)	48(6)
H(18A)	2022(13)	4517(19)	-954(13)	45(6)
H(18B)	2349(15)	4140(20)	-67(14)	54(7)
H(18C)	1831(13)	5300(20)	-253(12)	39(5)
H(19)	1758(10)	1271(15)	7(10)	15(4)
H(21)	1862(11)	-560(16)	-886(11)	23(4)
H(22)	2419(10)	-2566(16)	-1052(10)	21(4)
H(23)	3504(11)	-3590(16)	134(10)	23(4)
H(24)	3957(11)	-2568(17)	1419(10)	22(4)
H(26)	4512(11)	-1230(16)	2517(10)	21(4)
H(27A)	3203(14)	-1430(20)	3104(13)	45(6)
H(27B)	4033(13)	-2254(19)	3437(13)	41(6)
H(27C)	3358(12)	-2502(19)	2529(12)	35(5)
H(28A)	4637(11)	1035(17)	2978(11)	23(4)
H(28B)	4799(14)	-10(20)	3761(13)	44(6)
H(28C)	3970(12)	687(17)	3361(11)	28(5)

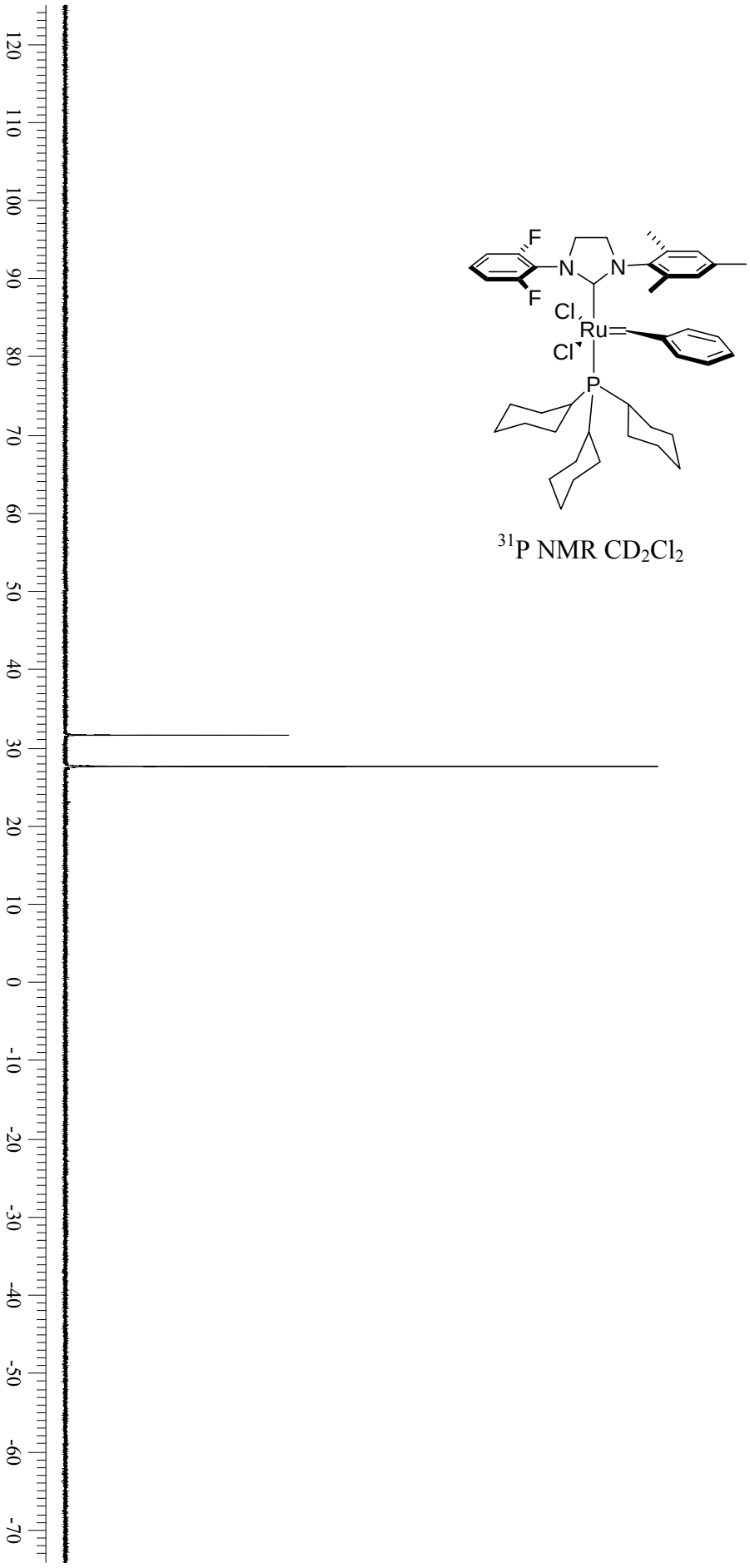
NMR Spectra



^{1}H NMR CD_2Cl_2



^{13}C NMR CD_2Cl_2



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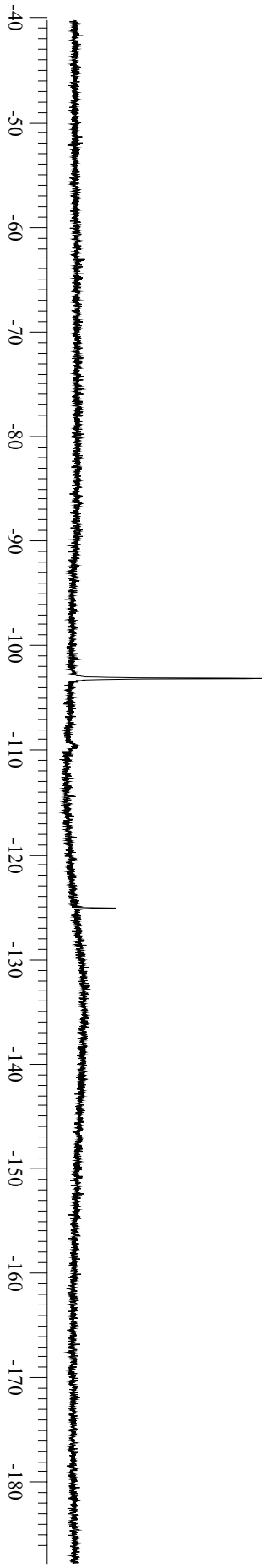

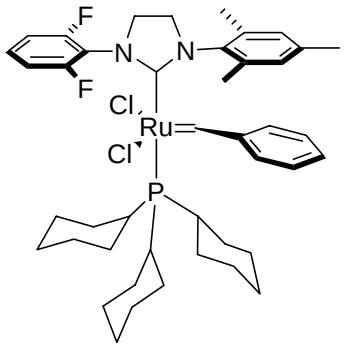

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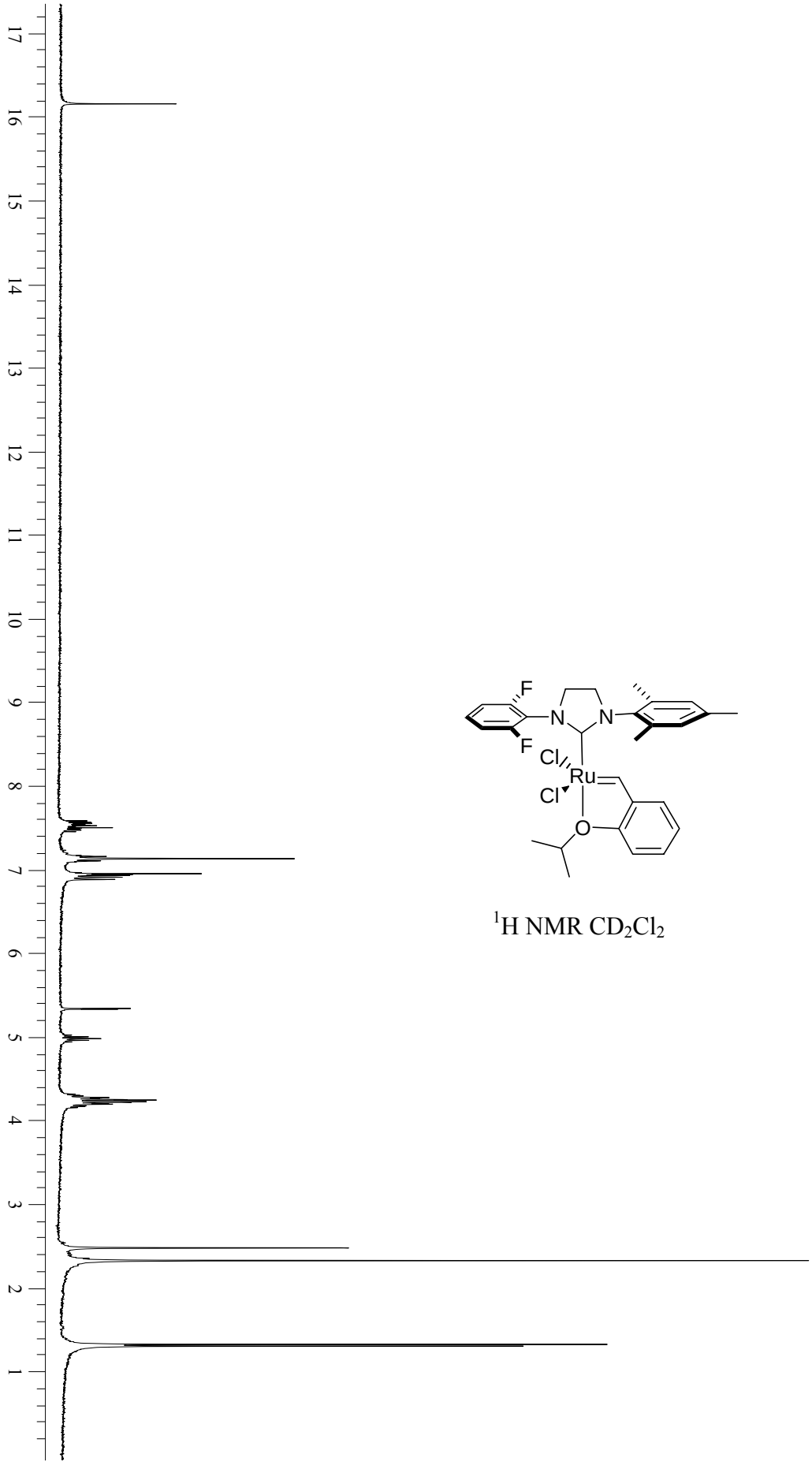

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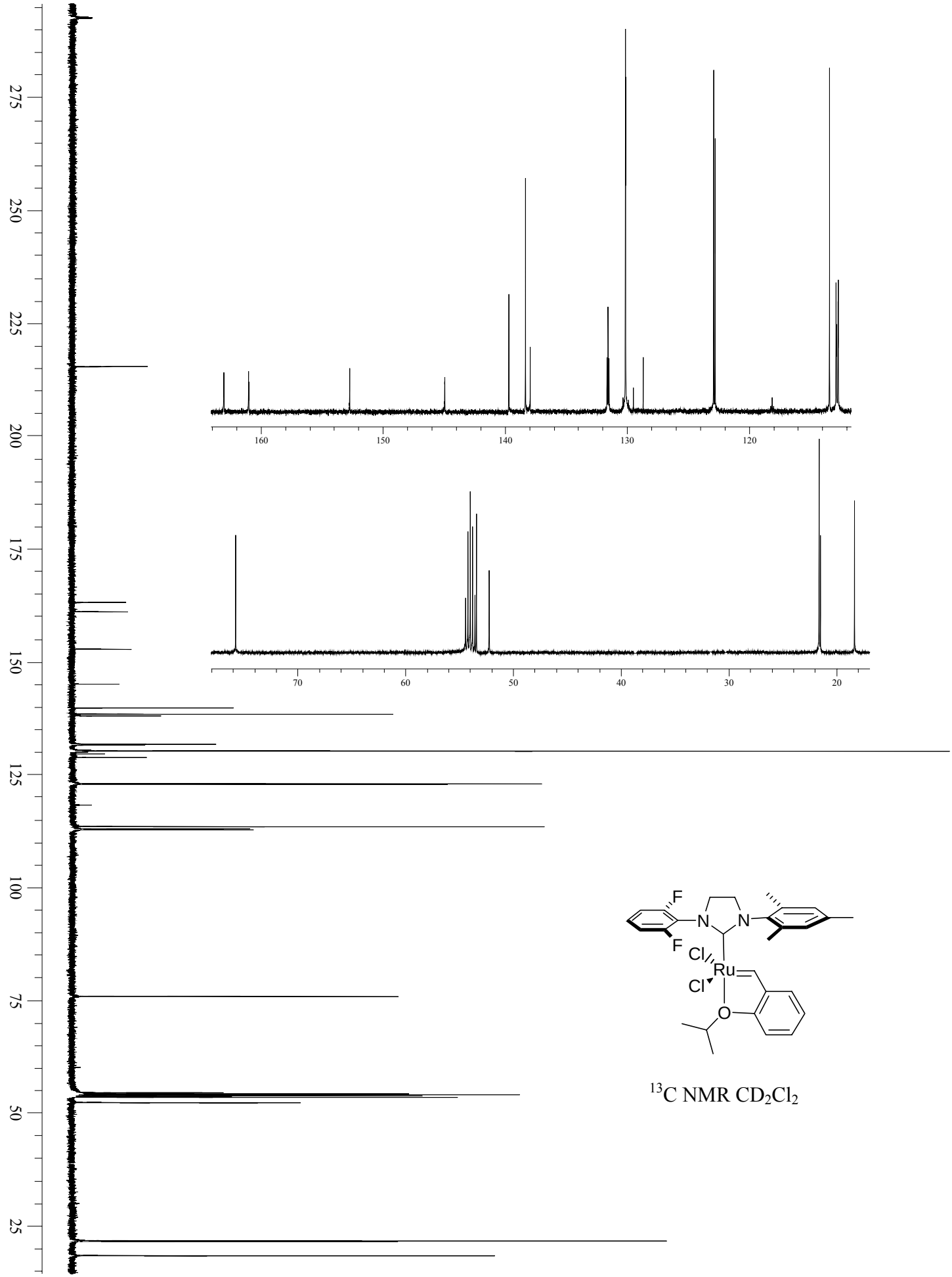

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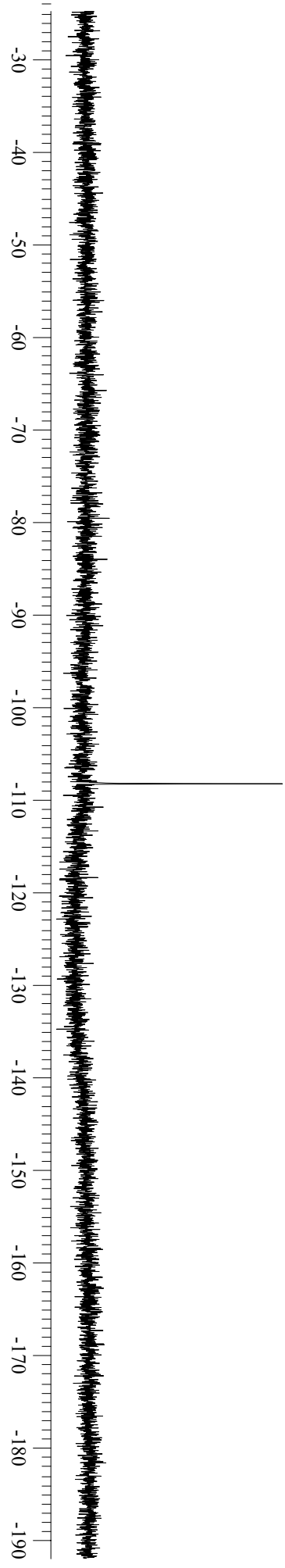

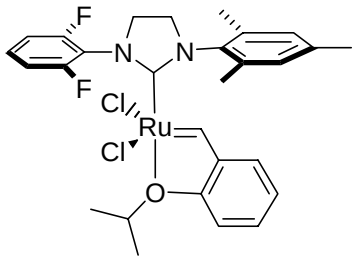

^{19}F NMR CD_2Cl_2